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Spatiotemporal heterogeneity and nonlinear drivers of carbon storage in the Pearl River Delta using GTWR and XGBoost-SHAP

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Abstract: Rapid urbanization reshapes regional carbon storage through interactions among natural conditions and human activities, however, the associated spatiotemporal nonstationarity, nonlinear responses, and factor interactions remain insufficiently understood. Taking the Pearl River Delta (PRD) urban agglomeration in China as a case study, this paper estimated the carbon storage from 2000 to 2023 using the InVEST model based on regional LUCC and analyzed their spatiotemporal evolution using GIS. Furthermore, a multidimensional indicator system covering vegetation, topography, human activities, and aridity was developed through robust multistage screening, and the GTWR and XGBoost-SHAP models were integrated to collaboratively identify the local spatiotemporal heterogeneity, global feature importance, nonlinear responses and interaction effects of driving factors, simultaneously capturing their spatiotemporal nonstationarity and complex nonlinear relationships. The results show that the dominant driving mechanism of carbon storage in the PRD has gradually shifted from the “terrain-vegetation protection-dominated” pattern to a composite mode featuring sustained vegetation support, weakened terrain constraints and intensified human disturbances. Vegetation acts as the strongest and most stable positive factor, with its marginal gain being most prominent in areas with moderate-to-low vegetation cover. Topography impacts diminish over time, and its restraining effect on land development declines. Human activity intensity exerts an increasingly strong negative non-linear influence with potential thresholds. Aridity plays a relatively weak role with insignificant spatiotemporal variations. Accordingly, priority should be given to protecting mountainous high-carbon-sink spaces, strictly controlling human-activity intensity in urban core areas and development fringes, and focusing on restoring regions with moderate-to-low vegetation cover.

Keywords: carbon storage, spatiotemporal heterogeneity, nonstationarity effects, GTWR, interpretable machine learning, Pearl River Delta

1. Introduction

Clarifying carbon storage dynamics driven by land-use and land-cover change (LUCC), particularly their responses to natural conditions and human activities, provides a critical scientific basis for assessing regional carbon balance, mitigating climate change, and advancing the Sustainable Development Goals (SDGs) (United Nations General Assembly 2015). In the rapidly urbanizing Pearl River Delta (PRD) urban agglomeration, China, land conversion and ecological degradation increasingly threaten ecosystem carbon retention. Characterizing the spatiotemporal heterogeneity and nonstationarity of carbon storage and identifying the core drivers are therefore critical for regional low-carbon spatial planning, effective ecological governance, and thus sustainability development.

Existing studies have extensively assessed LUCC-related carbon storage, especially using the Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) model (Tallis and Polasky 2009), which estimates carbon stored in aboveground biomass, belowground biomass, soil, and dead organic matter based on land-use-specific carbon densities (Zhao et al. 2023; Zhou et al. 2024b; Wang et al. 2022). Despite its operational simplicity and broad regional applicability, most InVEST-based studies emphasize land-use composition while inadequately addressing the joint effects of natural and socioeconomic drivers (García-Ontiyuelo et al. 2024; Dey et al. 2025; Sui et al. 2026; Wei et al. 2025). This limitation is particularly consequential in rapidly urbanizing regions, particularly in the PRD, where carbon storage is shaped by nonlinear interactions among topography, climate, vegetation, soils, population, and economic activity, causing the effects of individual drivers to vary considerably across space and time (Zeng and Sun 2024; Sui et al. 2026; Li et al. 2022). This requires methodological advances capable of disentangling the complex

nonlinear drivers of carbon storage. However, conventional global regression models such as ordinary least squares (OLS) generally assume linear and spatially stationary relationships, limiting their ability to capture the pronounced spatiotemporal heterogeneity and nonstationarity of human-environment interactions within urban agglomerations (Anselin 1988; Fotheringham et al. 2002; Ye et al. 2025); local-spatial econometric models such as Geodetector (Wang and Xu 2017) and multiscale geographically weighted regression (MGWR) (Oshan et al. 2019) can only interpret linear spatial differentiation (Song et al. 2026); machine-learning methods including random forest regression (Breiman 2001) are capable of capturing non-linear relationships yet lack the capacity to analyze temporal evolution.

Recent advances in spatiotemporal econometrics and interpretable machine learning offer effective tools for addressing these limitations. Geographically and temporally weighted regression (GTWR) models spatiotemporal nonstationarity by allowing regression coefficients to vary across both space and time (Huang et al. 2010; Fotheringham et al. 2017). It has been applied to estimate the spatially and temporally varying effects of urbanization, topography, and climate on ecosystem services (Wang et al. 2021). In parallel, XGBoost, an extreme gradient-boosting algorithm, can capture complex nonlinear relationships while maintaining strong predictive performance (Breiman 2001; Chen and Guestrin 2016). When combined with SHapley Additive exPlanations (SHAP), it also provides interpretable estimates of global and observation-specific predictor contributions (Lundberg and Lee 2017). Complementary tools such as partial dependence plots (PDPs) further facilitate the identification of nonlinear responses, potential thresholds, and interaction patterns (Friedman 2001). The combined use of GTWR and XGBoost-SHAP is therefore methodologically complementary. GTWR quantifies spatiotemporal heterogeneity, whereas XGBoost-SHAP characterizes nonlinear marginal effects, relative predictor contributions, and multivariate interactions. This integrated framework enables carbon-storage drivers to be examined from both spatial-temporal and predictive perspectives, thereby providing a more comprehensive basis for interpreting differentiated associations among natural, social, and economic factors.

However, existing studies of carbon-storage drivers have largely relied on static linear models, including multiple linear and spatial regression, or have used machine-learning methods independently or in relatively simple combinations (Seto et al. 2012; Eigenbrod et al. 2011; Guo et al. 2026; Zhang et al. 2025; Zhou et al. 2024a; Li and Li 2025). A framework that simultaneously integrates systematic driver identification, spatiotemporal heterogeneity, nonlinear responses, and predictor interactions remains underdeveloped. Moreover, previous research has focused primarily on natural systems, such as wetlands, forests, and river basins (Wei et al. 2025; Ye et al. 2025; Song et al. 2026; García-Ontiyuelo et al. 2024; Liu et al. 2019). Few studies have examined how natural, social, and economic factors jointly shape carbon storage through spatially and temporally varying and nonlinear processes in highly urbanized urban agglomerations.

Accordingly, this study uses long-term LUCC data for the PRD (2000-2023) to estimate terrestrial carbon storage with the InVEST model and characterize its spatial and temporal dynamics in a GIS environment. County- and district-level administrative units serve as the basic analytical units. Variance inflation factors (VIFs) are used to diagnose multicollinearity, while random forest regression (RFR) and principal component analysis (PCA) support predictor screening and redundancy reduction (Dormann et al. 2013). Based on these procedures, a multidimensional indicator system is developed to represent vegetation, topography, human-activity intensity, and aridity. GTWR and XGBoost-SHAP are then integrated to examine the drivers of carbon storage from complementary perspectives, including spatiotemporal heterogeneity, nonlinear responses, and interaction effects. The results are expected to inform differentiated carbon management, ecological restoration, and low-carbon territorial planning in the PRD, while providing a transferable methodological framework for carbon-cycle research in comparable megacity regions in China and elsewhere.

2. Materials and Methods

2.1 Study area

The PRD urban agglomeration, located in south-central Guangdong Province, covers

approximately 54,000 km² and comprises nine prefecture-level cities (Figure 1). In 2023, it accommodated 78.6 million residents, generated over CNY 12 trillion in GDP, and reached an urbanization rate of 87.5%. The PRD constitutes the core of the Guangdong-Hong Kong-Macao Greater Bay Area, one of China's most densely populated and economically dynamic regions.

The PRD has a subtropical monsoon climate, with mean annual temperatures of 21-23 °C and solar radiation of 4,200-5,400 MJ/m². Its central alluvial plain is predominantly below 50 m in elevation and is bordered by hills, mountains, and islands (Figure 1). Lateritic red and paddy soils support intensive agriculture, while monsoon evergreen broad-leaved forest constitutes the dominant natural vegetation. The Xijiang, Beijiang, and Dongjiang rivers converge within a dense river network before discharging through eight major estuaries, creating extensive wetland systems.

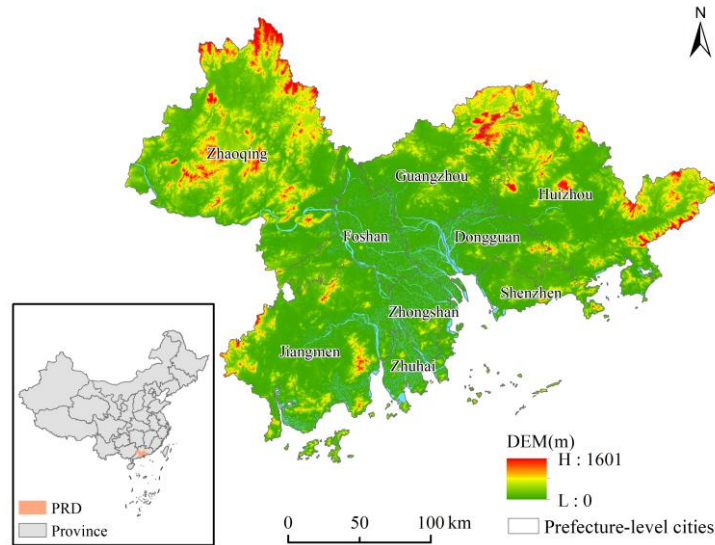


Figure 1 Study area

2.2 Data sources and preprocessing

This study compiled annual raster datasets on LUCC, ecological conditions, and socioeconomic factors in the PRD for 2000-2023 (Table 1), obtained from the Registration and Publication System for Resources and Environmental Science Data (<https://www.resdc.cn/>) and the National Tibetan Plateau Data Center (<https://data.tpdc.ac.cn/home>). The original 26 land-use classes were reclassified into six categories consistent with the global LUCC classification system (Table 2). All raster layers were projected, resampled, and spatially aligned in ArcGIS at a 30-m resolution.

The analysis covered 48 county- and district-level units; Dongguan and Zhongshan were each treated as a single prefecture-level unit. A five-dimensional indicator system was established to represent the natural and socioeconomic determinants of carbon storage (Table 3). Topographic factors included elevation and aspect, with aspect derived from the DEM and summarized as the proportions of sun-facing and shaded slopes. Climate was characterized by mean annual precipitation and potential evapotranspiration, while vegetation and soil conditions were represented by the normalized difference vegetation index and clay content, respectively. Socioeconomic indicators comprised GDP, population density, and nighttime-light intensity.

Before model estimation, variance inflation factor (VIF) analysis, RFR, PCA, and robustness checks were conducted to diagnose multicollinearity, screen predictors, and minimize information redundancy. The resulting GTWR-XGBoost-SHAP framework was implemented in GWmodels 2.0 and Python to examine the spatiotemporal heterogeneity, nonlinear responses, and interaction effects of carbon-storage drivers in the PRD during 2000-2023.

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Table 1 Sources of raw raster datasets and relative public database (URL)

Type	Data	Resolution (m)	Source
LUC	China multi-period land use remote sensing monitoring dataset	30	Registration and Publication System for Resources and Environmental Science Data (https://www.resdc.cn/DOI/DOI.aspx?DOIID=201)
Ecological conditions	DEM	30	Registration and Publication System for Resources and Environmental Science Data (https://www.resdc.cn/data.aspx?DATAID=217)
	Normalized Difference Vegetation Index (NDVI)	30	Registration and Publication System for Resources and Environmental Science Data (https://www.resdc.cn/DOI/DOI.aspx?DOIID=68 ;
	Annual Potential Evapotranspiration (PET)	500	https://www.resdc.cn/data.aspx?DATAID=365)
	Mean Annual Precipitation (MAP)	1000	National Qinghai-Tibet Plateau Science Data Center (https://data.tpd.ac.cn/zh-hans/data/faae7605-a0f2-4d18-b28f-5cee413766a2)
Socioeconomic factors	Soil type	1000	Registration and Publication System for Resources and Environmental Science Data (https://www.resdc.cn/data.aspx?DATAID=260)
	GDP	1000	Registration and Publication System for Resources and Environmental Science Data (https://www.resdc.cn/DOI/DOI.aspx?DOIID=33 ;
	Population density	1000	https://www.resdc.cn/DOI/DOI.aspx?DOIID=32 ;
	Nighttime light intensity	500	https://www.resdc.cn/DOI/DOI.aspx?DOIID=105)

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Table 2 Re-class of LUC

Code	Major category	Included classes
1	Cultivated land (CL)	paddy field, dry land
2	Forest land (FL)	forested land, shrubland, sparse forest land, other forest land
3	Grassland (GL)	High, medium, and low coverage grasslands
4	Water bodies (W)	rivers, lakes, reservoirs and ponds, permanent glaciers and snowfields, tidal flats, beaches
5	Construction land (ConL)	Urban land, rural residential areas, other construction land
6	Unused land (UL)	desert, gobi, saline-alkali land, swamp, bare land, bare rock, texture, other

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Table 3 Evaluation indicator system for carbon storage

Dimension	Indicator	Unit
Topographical Conditions	Elevation	m
	Aspect	
	Proportion of sunny slope (P_SunS)	%
Climatic Conditions	Proportion of shady slope (P_Shds)	%
	Mean annual precipitation (MAP)	mm
	Potential evapotranspiration (PET)	mm
Vegetation Ecology	Normalized difference vegetation index (NDVI)	\
Soil Properties	Proportion of clay (P_Clay)	%
Socioeconomic Activities	GDP	100 million yuan/km ²
	Population density (Pop_Dens)	10000 people/km ²
	Nighttime Light Intensity (NLI)	DN/km ²

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2.3 Methods

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2.3.1 Land use transfer matrix

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The land-use transition matrix quantifies the magnitude and direction of conversions among land-use categories over a given period, as follows:

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$$S_{n \times n} = \begin{pmatrix} S_{11} & \cdots & S_{1j} \\ \vdots & \ddots & \vdots \\ S_{i1} & \cdots & S_{ij} \end{pmatrix} \quad (i = 1, 2, \dots, n; j = 1, 2, \dots, n) \quad (1)$$

where S_{ij} denotes the area converted from land use category i to category j during the study period. When $i=j$, it represents the area where land category i remains unchanged. The variable n is the total number of land-use categories.

2.3.2 VIF analysis, Pearson's correlation and PCA

VIFs were used to assess multicollinearity among predictors in the multiple regression model. The VIFs for predictor j is calculated as follows:

$$\text{VIF}_j = \frac{1}{1 - R_j^2} \quad (2)$$

where R_j^2 is obtained by regressing x_j on all other explanatory variables. As R_j^2 approaches 1, x_j is increasingly explained by a linear combination of the other predictors, leading to a higher VIF value and greater uncertainty in its estimated coefficient. Following commonly used guidelines, VIF values below 5 indicate low multicollinearity, values between 5 and 10 suggest potentially substantial multicollinearity, and values above 10 indicate severe multicollinearity (Hair et al. 2011; Dormann et al. 2013).

Pearson's correlation coefficient (r) measures the strength and direction of the linear association between two continuous variables and ranges from -1 to 1 (Cohen 1988). As it captures only pairwise linear relationships, it was used as a preliminary diagnostic of correlations among explanatory variables, complementing the VIF analysis and informing subsequent variable selection.

PCA is a linear dimensionality-reduction technique that transforms correlated variables into a smaller set of orthogonal principal components. The first component determines the maximum variance in the data, while each subsequent component explains the greatest remaining variance subject to orthogonality constraints. Retaining components with a high cumulative explained variance reduces dimensionality and multicollinearity while preserving most of the original information.

2.3.3 RFR and auxiliary interpretation methods

RFR combines multiple decision trees to improve predictive accuracy and generalizability (Breiman 2001). Its prediction for explanatory-variable vector x is

$$\hat{y}(x) = \frac{1}{B} \sum_{b=1}^B T_b(x) \quad (3)$$

where B is the number of trees, and $T_b(x)$ is the prediction from tree b . Each tree is fitted to a bootstrap sample, and a random subset of predictors is considered at each split, reducing correlations among trees.

To construct the RFR model, the data were partitioned into training and test sets for model fitting and out-of-sample evaluation, respectively. Predictive performance was quantified using the coefficient of determination (R^2), root mean squared error (RMSE), and mean absolute error (MAE):

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (4)$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (5)$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (6)$$

where n is the test set size; y_i and $\hat{y}_i$ are the observed and predicted values; and $\bar{y}$ is the mean of the observed value. Better performance is indicated by higher R^2 and lower RMSE and MAE.

Sensitivity to training-sample variation was assessed through 5,000 bootstrap iterations. In each iteration, the RFR model was refitted to a resample of the training data, and test-set performance metrics and feature-importance scores were recorded (Strobl et al. 2007). Percentile-based 95% confidence intervals were calculated as

$$\text{CI}_{95\%}(Q) = [Q_{0.025}^*, Q_{0.975}^*] \quad (7)$$

where Q^* denotes the bootstrap estimate of Q , and $Q_{0.025}^*$ and $Q_{0.975}^*$ are the corresponding percentiles of the bootstrap distribution (Efron and Tibshirani 1997; Wager et al. 2014). Larger importance scores indicate greater relative predictive contributions within the fitted model.

As feature importance does not indicate effect direction, PDPs were used to characterize marginal model responses (Friedman 2001):

$$\hat{P}_j(x_j) = \frac{1}{n} \sum_{i=1}^n \hat{f}(x_j, x_{x,-j}) \quad (8)$$

where $\hat{P}_j(x_j)$ denotes the partial dependence of predictor j at a given value x_j ; $\hat{f}$ is the fitted model and $x_{x,-j}$ contains all predictors except j ; and n is the number of samples. PDPs reveal the average direction and form of model-predicted associations, including nonlinearities and potential turning points, but should not be interpreted as causal effects.

2.3.4 InVEST model

The InVEST model evaluates terrestrial carbon storage by analyzing the spatial distribution of land use categories and their corresponding carbon density data. The formula is presented below:

$$C_i = C_{i\text{-above}} + C_{i\text{-below}} + C_{i\text{-dead}} + C_{i\text{-soil}} \quad (9)$$

$$C_{i\text{-total}} = \sum_{i=1}^n C_i \times A_i \quad (10)$$

where C_i denotes the terrestrial carbon stock of land use category i ; $C_{i\text{-above}}$ represents the aboveground carbon density; $C_{i\text{-below}}$ indicates the underground carbon density; $C_{i\text{-dead}}$ stands for the dead organic matter carbon density; $C_{i\text{-soil}}$ represents the soil organic matter carbon density; $C_{i\text{-total}}$ is the total terrestrial carbon stock; A_i denotes the area of land use category i ; n is the total number of land use categories. Due to the extremely low content of $C_{i\text{-dead}}$ and data availability constraints, this study excluded it from consideration.

Under identical climatic conditions, carbon density exhibits minimal variation across land use categories at the regional scale. Based on existing studies (Zhu et al. 2021; Wu et al. 2016; Li and Li 2025; Zhang et al. 2025), the carbon density values for each land use category identified in this study are presented in Table 4.

Table 4 Carbon density of each land use category (t/km²)

Land use	$C_{i\text{-above}}$	$C_{i\text{-below}}$	$C_{i\text{-soil}}$
CL	13.50	2.70	17.34
FL	58.30	14.58	19.73
GL	3.01	13.53	16.00
W	0.21	0.00	0.00
ConL	1.20	0.93	12.48
UL	2.10	0.00	11.36

2.3.4 GTWR model

Geographically and temporally weighted regression (GTWR) extends the conventional

geographically weighted regression (GWR) framework by incorporating temporal information into the spatial weighting scheme, thereby capturing spatial non-stationarity and temporal variation in covariate effects (Huang et al. 2010). Unlike global models with constant coefficients, GTWR estimates a local regression for each district-year observation, allowing coefficients to vary across longitude, latitude, and time. The model is specified as follows:

$$y_{it} = \beta_0(\mu_i, v_i, t_i) + \sum_{k=1}^p \beta_k(\mu_i, v_i, t_i) x_{ikt} + \varepsilon_{it} \quad (11)$$

where y_{it} denotes carbon stock of district i in year t ; (μ_i, v_i, t_i) represents its spatiotemporal coordinates; $\beta_0(\cdot)$ is the local intercept; $\beta_k(\cdot)$ refers to the spatiotemporally varying coefficient of predictor k ; x_{ikt} is the corresponding predictor value; ε_{it} is the random error; and p is the number of predictors.

The local coefficient vector at each sample is estimated via weighted least squares:

$$\hat{\beta}(\mu_i, v_i, t_i) = [X^T W(\mu_i, v_i, t_i) X]^{-1} X^T W(\mu_i, v_i, t_i) y \quad (12)$$

where $\hat{\beta}(\mu_i, v_i, t_i)$ denotes the vector of local regression coefficients at location i , including the local intercept and the coefficient of each explanatory variable; X is the matrix of explanatory variables; y is the vector of dependent-variable observations; and $W(\mu_i, v_i, t_i)$ is the diagonal spatiotemporal weight matrix for location i , constructed using a Gaussian kernel such that the weights decrease with increasing spatial and temporal distances from the target observation.

Following model estimation, an adaptive bandwidth was selected by minimizing the cross-validation criterion or corrected Akaike information criterion (AICc) (Fotheringham et al. 2017; Fotheringham et al. 2015). Local R^2 , coefficient estimates (including the intercept), and associated t -statistics were extracted to evaluate local model fit and the significance of spatiotemporally varying effects.

2.3.5 XGBoost-SHAP

XGBoost is a regularized gradient-boosted decision-tree ensemble capable of modeling nonlinear relationships, threshold effects, and interactions among multidimensional drivers of carbon stocks (Chen and Guestrin 2016). Its objective function combines squared-error loss with a complexity penalty:

$$\hat{y} = \sum_{k=1}^K f_k(x_i), f \in Z \quad (13)$$

$$\Gamma(\phi) = \sum_{i=1}^n l(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (14)$$

where y_i and $\hat{y}_i$ denote the actual observed value and the model's predicted value for sample i aggregated across K trees, respectively; Z is the function-space tree for regression trees; $l(\cdot)$ is the squared-error loss. The regularization term for tree f_k is $\Omega(f_k) = \gamma T + 1/2(\lambda \|\omega\|)$, where T denotes the number of leaves, ω is the leaf-weight vector, and γ and λ are penalize model complexity to reduce overfitting. Hyperparameters were optimized using grid search with five-fold cross-validation.

As conventional XGBoost importance measures do not convey effect direction or explicitly quantify interactions, SHAP analysis was used to assess global importance, sample-specific contributions, and pairwise interactions (Lundberg and Lee 2017). For observation i ,

$$\hat{f}(x_i) = g(\phi_0) + \sum_{k=1}^p \phi_{ik} \quad (15)$$

where $\hat{f}(x_i)$ is the model's predicted value for sample i ; $g(\phi_0)$ is the baseline prediction (the expected predicted carbon stock), and ϕ_{ik} denotes the SHAP value of predictor k for sample i . Positive and negative SHAP values indicate that a predictor increases or decreases the prediction relative to this baseline, respectively. The SHAP value is defined as:

$$\phi_{ik} = \sum_{S \subseteq \{1, \dots, p\} \setminus \{k\}} \frac{|S|(p - |S| - 1)}{p} [v_i(S \cup \{k\}) - v_i(S)] \quad (16)$$

where S represents any feature subset excluding variable k , $|S|$ is model prediction under feature combination S . $v_i(S)$ denotes the expected model output for sample i when only the subset of variables S is considered.

SHAP interaction values were calculated to separate main effects from pairwise interactions. For predictors j and k , the off-diagonal interaction value $\phi_{i,jk}$ is symmetric ($\phi_{i,jk}=\phi_{i,kj}$) and represents their interaction contribution, whereas the diagonal term represents the main effect after accounting for interactions with other predictors:

$$\phi_{i,jk} = \sum_{S \subseteq \{1, \dots, p\} \setminus \{k\}} \frac{|S|(p-|S|-1)}{2p(-1)} \Delta_{i,jk}(S), j \neq k \quad (17)$$

$$\Delta_{i,jk}(S) = v_i(S \cup \{j, k\}) - v_i(S \cup \{j\}) - v_i(S \cup \{k\}) + v_i(S) \quad (18)$$

where $\Delta_{i,jk}(S)$ denotes the difference between the change in the model prediction when variables j and k are added jointly to subset S and the sum of their respective contributions when added separately. Overall interaction strength was quantified as:

$$I_{jk}^{\text{int}} = \frac{1}{n} \sum_{i=1}^n |\phi_{i,jk}| \quad (19)$$

Higer I_{jk}^{int} values indicate stronger model-based interaction. Signed interaction values indicate whether a given interaction increases or decreases the prediction relative to an additive-effects specification.

3. Results and analysis

3.1 Land-use spatiotemporal evolution

Table 5 summarizes LUCC in the PRD from 2000 to 2023 across cultivated land (CL), forest land (FL), grassland (GL), water bodies (W), construction land (ConL), and unused land (UL). Forest and cultivated land remained the dominant categories, whereas unused land accounted for the smallest share. Construction land recorded the largest net increase, expanding by 3,550.64 km² (102.90%), while cultivated land and water bodies declined substantially.

Land-use transitions varied across periods. During 2000-2005, cultivated land decreased by 1,118.21 km², nearly offsetting the 1,117.91 km² expansion of construction land. Between 2005 and 2010, cultivated land declined by a further 1,647.68 km², while construction and forest land increased by 990.46 and 663.12 km², respectively, reflecting simultaneous urban expansion and ecological restoration. From 2010 to 2015, water bodies decreased by 379.74 km² as construction-land expansion moderated. During 2015-2020, cultivated and construction land increased at the expense of the other categories. Between 2020 and 2023, cultivated and construction land expanded by 440.80 and 216.19 km², respectively, whereas water bodies and forest land decreased by 507.36 and 140.37 km². Overall, although cultivated-land protection policies periodically slowed its decline, cultivated land in 2023 remained 11.88% below its 2000 level.

Table 5 Land-use changes in the PRD from 2000 to 2023

Year	Area/Proportion	CL	FL	GL	W	ConL	UL
2000	Area (km ²)	17459.61	29306.05	74.40	4200.33	3450.46	5.66
	Proportion (%)	32.04	53.78	0.14	7.71	6.33	0.01
2005	Area (km ²)	16341.40	29172.02	121.93	4287.17	4568.37	5.61
	Proportion (%)	29.99	53.53	0.22	7.87	8.38	0.01
2010	Area (km ²)	14693.72	29805.15	99.02	4325.23	5558.85	14.54
	Proportion (%)	26.96	54.69	0.18	7.94	10.20	0.03
2015	Area (km ²)	14291.40	30031.62	57.55	3945.49	6154.27	16.18
	Proportion (%)	26.22	55.11	0.11	7.24	11.29	0.03
2020	Area (km ²)	14945.03	29341.63	32.36	3374.59	6784.91	17.98
	Proportion (%)	27.42	53.84	0.06	6.19	12.45	0.03
2023	Area (km ²)	15385.84	29201.26	24.71	2867.23	7001.10	16.38
	Proportion (%)	28.23	53.58	0.05	5.26	12.85	0.03

Table 6 identifies the principal LUCC pathways in the PRD during 2000-2023. Cultivated

land had the largest gross outflow (5,109.05 km²), mainly to forest and construction land, consistent with ecological restoration and urban expansion. Forest loss totaled 2,054.45 km², of which 88.15% was converted to cultivated land, revealing substantial reciprocal conversion between these categories. Construction land showed the largest net gain, receiving 3,587.39 km² while losing only 36.75 km² (a ratio of approximately 98:1). Cultivated land accounted for 79.10% of construction-land gains, although this pathway weakened as farmland protection intensified. Water bodies also experienced considerable conversion (1,186.26 km²) became cultivated land and 486.80 km² became construction land, indicating agricultural reclamation and urban encroachment. Changes involving grassland and unused land were comparatively limited.

Figure 2 shows that construction land expanded outward from major urban centers, especially Guangzhou, Shenzhen, Foshan, Dongguan, and Zhongshan. Development shifted from dispersed, low-density growth in 2000-2005 to intensified peripheral expansion and increasingly contiguous built-up areas during 2005-2015, largely replacing cultivated land. Forest land remained concentrated in Zhaoqing, Jiangmen, and Huizhou, whereas water bodies clustered along major rivers and pond systems. During 2015-2023, extensive pond conversion, particularly in the traditional aquaculture areas of Foshan and Zhongshan, further reduced water coverage.

Above results implied that LUCC was dominated by urban expansion, cultivated-land loss, reciprocal conversion between cultivated and forest land, and water-body contraction.

Table 6 Land-use transfer matrix in the PRD from 2000 to 2023 (km²)

Land use	CL	FL	GL	W	ConL	UL	Total (out-transfer area)
CL	—	1924.26	11.80	328.59	2837.74	6.66	5109.05
FL	1811.09	—	7.28	11.21	223.89	0.99	2054.45
GL	23.27	4.95	—	6.48	36.80	0.68	72.17
W	1186.26	19.88	3.09	—	486.80	7.42	1703.46
ConL	13.83	0.53	0.05	22.32	—	0.02	36.75
UL	0.83	0.04	0.26	1.75	2.17	—	5.05
Total (in-transfer area)	3035.27	1949.66	22.49	370.35	3587.39	15.77	—

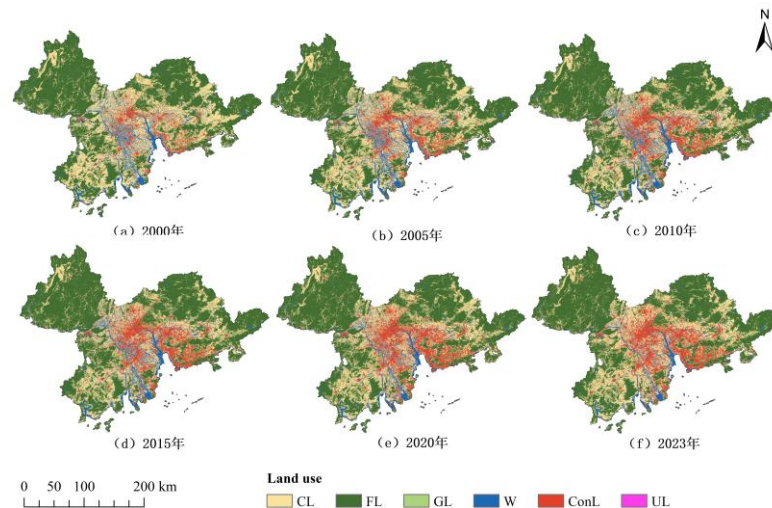


Figure 2 Land-use spatial patterns from 2000-2023

3.2 Spatiotemporal dynamics of carbon storage

Table 7 presents InVEST-based estimates of carbon storage in the PRD from 2000 to 2023.

Regional carbon storage remained broadly stable, with only minor fluctuations, owing to the dominance and relatively high carbon densities of forest and cultivated land. By 2023, these two land-use types accounted for 96.87% of the total carbon storage, while all other categories contributed less than 4%.

Table 8 further shows that carbon-storage losses in the PRD totaled 8.12×10^6 t from 2000 to 2023, primarily due to the conversion of cultivated and forest land to construction land. Despite substantial losses of water bodies, their low carbon density resulted in a limited effect on total carbon storage. Meanwhile, land-use transitions associated with construction-land expansion generated an estimated gain of 5.20×10^6 t, potentially reflecting the conversion of low-carbon-density unused land and the incorporation of urban green space. However, this gain did not offset losses from cultivated and forest land, resulting in a net decline of 2.91×10^6 t from 2000-2023 and underscoring the importance of land-use allocation in regional carbon management.

Figure 3 reveals a pronounced center-periphery pattern of regional carbon storage, with low storage in the highly urbanized central PRD and high in its mountainous margins. Particularly, Guangzhou, Foshan, Dongguan, Shenzhen, and Zhongshan contain extensive built-up land, dense populations, and concentrated infrastructure, resulting in relatively low carbon-storage capacity. In contrast, the forest-dominated northwestern, northeastern, and southeastern areas constitute the region's principal carbon-stock reservoirs.

Table 7 Carbon storage from 2000 to 2023 (1×10^4 t)

Year	CL	FL	GL	W	ConL	UL	Total
2000	5855.95	27140.33	24.21	8.82	504.11	0.76	33534.18
2005	5480.91	27016.21	39.67	9.00	667.44	0.76	33213.99
2010	4928.27	27602.54	32.22	9.08	812.15	1.96	33386.22
2015	4793.34	27812.28	18.73	8.29	899.14	2.18	33533.96
2020	5012.56	27173.28	10.53	7.09	991.28	2.42	33197.16
2023	5160.41	27043.28	8.04	6.02	1022.86	2.20	33242.81

Table 8 Carbon stock changes from 2000 to 2023

Period	Area/carbon stock	Land use type						Gain	Loss	Net change
		CL	FL	GL	W	ConL	UL			
2000-2005	Area (km ²)	-1118.21	35.58	-42.03	-825.75	3334.46	12.32	/	/	/
	Carbon stock (10 ⁴ t)	-375.05	32.95	-13.68	-1.73	487.16	1.66	521.77	-390.46	131.31
2005-2010	Area (km ²)	-1647.68	633.12	-22.91	38.06	990.47	8.94	/	/	/
	Carbon stock (10 ⁴ t)	-552.63	209.74	-13.49	-0.80	86.99	0.22	296.95	-566.92	-269.97
2010-2015	Area (km ²)	-402.32	226.47	-41.46	-379.74	595.42	1.63	/	/	/
	Carbon stock (10 ⁴ t)	-134.94	209.74	-13.49	-0.80	86.99	0.22	296.95	-149.23	147.72
2015-2020	Area (km ²)	653.63	-689.99	-25.19	-570.90	630.65	1.80	/	/	/
	Carbon stock (10 ⁴ t)	219.23	-639.00	-8.20	-1.20	92.14	0.24	311.61	-648.40	-336.79
2020-2023	Area (km ²)	440.80	-140.37	-7.65	-507.36	216.18	-1.61	/	/	/
	Carbon stock (10 ⁴ t)	147.85	-130.00	-2.49	-1.07	31.58	-0.22	179.43	-133.78	45.65
2000-2023	Area (km ²)	-2073.78	-104.79	-49.68	-1333.11	3550.64	10.72	/	/	/
	Carbon stock (10 ⁴ t)	-695.54	-97.05	-16.17	-2.80	518.75	1.44	520.19	-811.56	-291.37

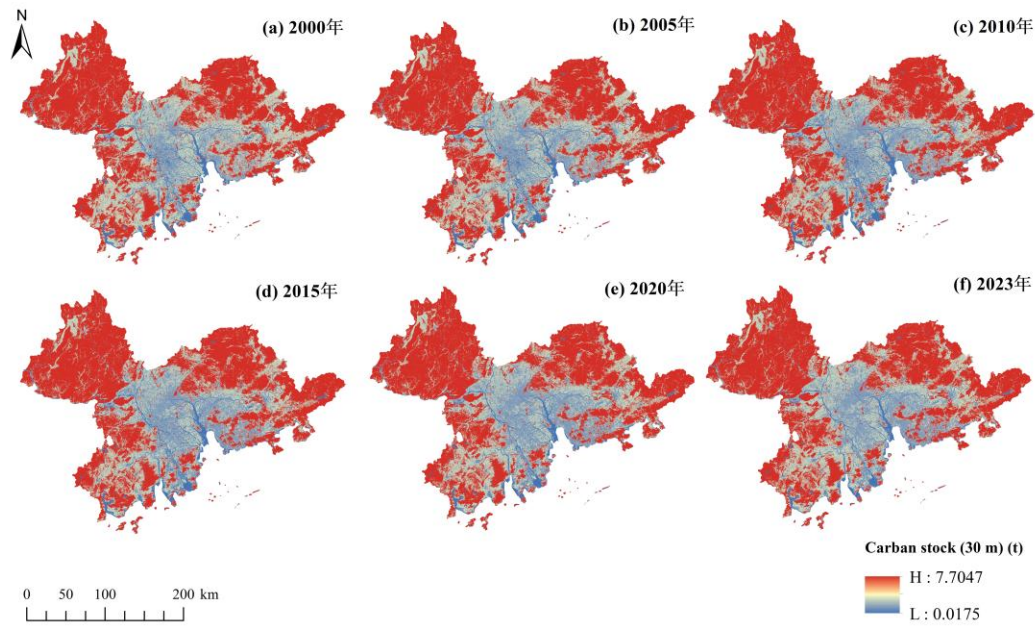


Figure 3 Spatiotemporal patterns of carbon storage from 2000 to 2023

3.3 Identification of drivers for carbon storage

Using district- and county-level panel data for the PRD (2000-2023), carbon storage (CS) was modeled against ten predictors spanning five dimensions across topography, climate, vegetation, soil properties, and socioeconomic activity (Table 3). Key predictors were screened using an integrated framework comprising VIFs, Pearson correlations, PCA, RFR, and PDPs.

3.3.1 VIFs and Pearson correlation

VIFs and Pearson correlations were examined to assess predictor redundancy, which can bias random-forest feature-importance estimates. As shown in Figure 4, all VIFs were below 10; NDVI had the highest value (8.2), whereas all others were below 6, indicating moderate but not severe multicollinearity. Correlations were generally moderate within predictor dimensions and weak across dimensions. GDP, Pop_Dens, and NLI were significantly and positively correlated, reflecting the spatial co-occurrence of economic activity, population concentration, and urban development.

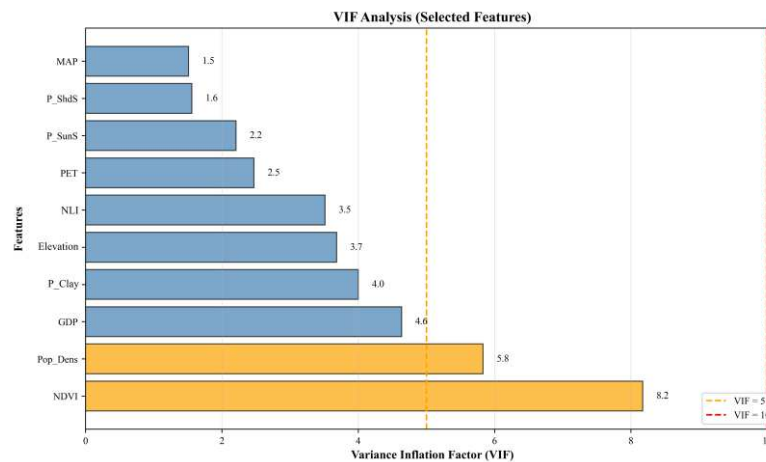


Figure 4 VIF tests for ten predictors

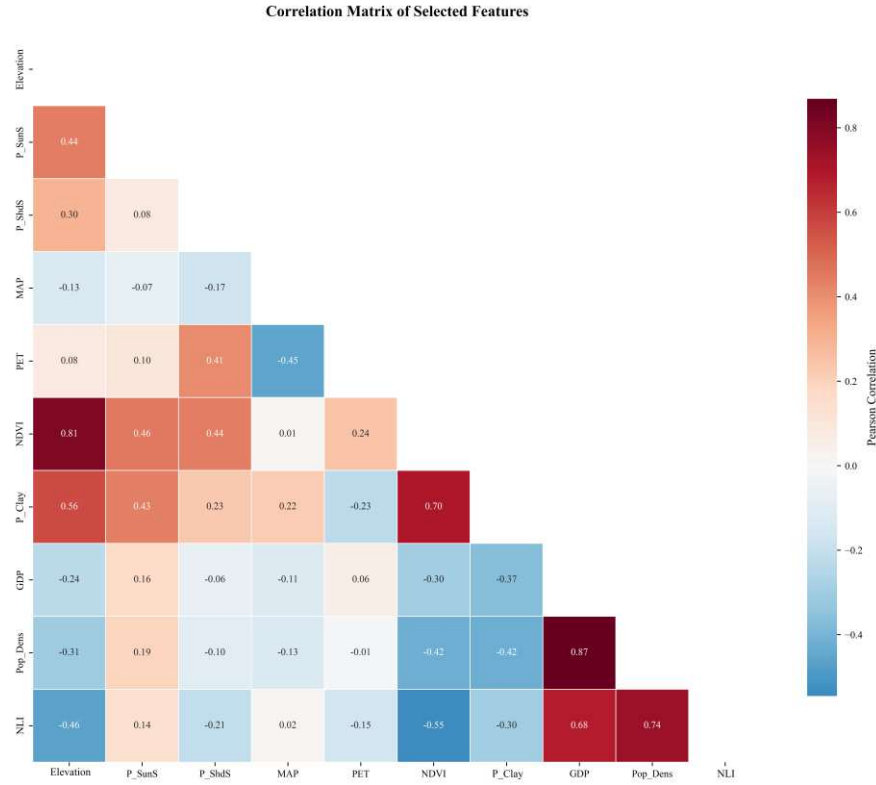
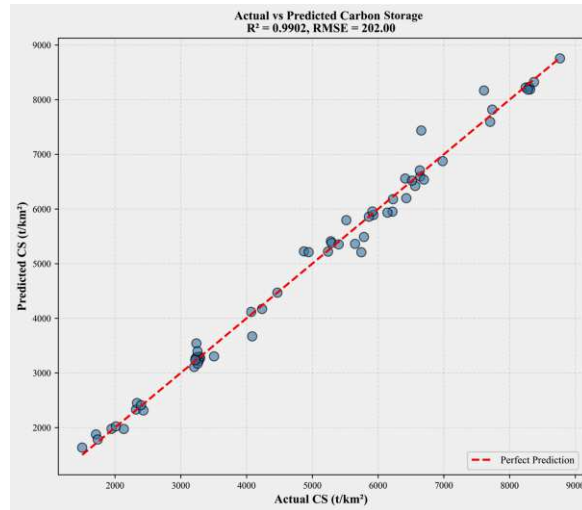


Figure 5 Pearson correlation coefficients for ten predictors

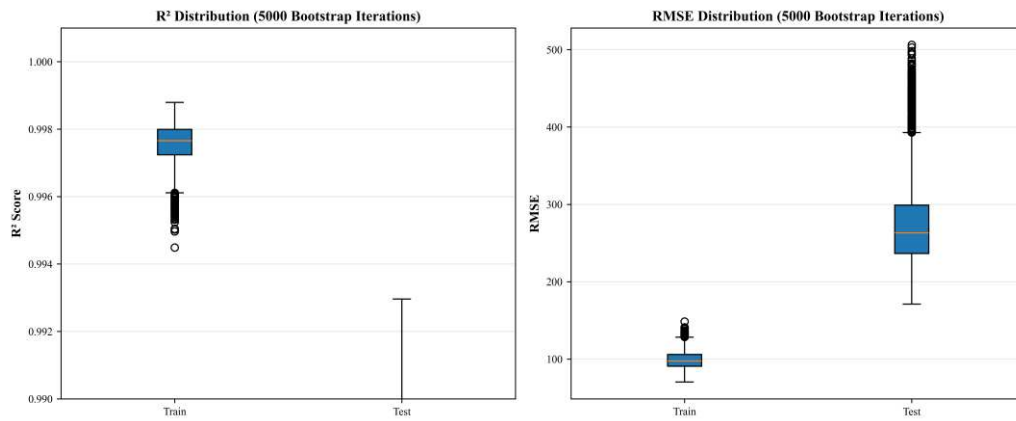
3.3.2 Random forest regression

Using district/county-level carbon storage as the response variable and the ten indicators as predictors, we trained a RFR model and evaluated it using a train-test split, cross-validation, and 5,000 bootstrap iterations. The model performed strongly, achieving an R^2 of 0.997 and an RMSE of 102.82 t/km² on the training set, compared with an R^2 of 0.9902, an RMSE of 202.00 t/km², and an MAE of 134.41 t/km² on the test set (Figure 6(a)). Cross-validation (CV) produced with an R^2 of 0.985. Bootstrap results further supported model stability, with mean training- and test-set R^2 values of 0.997 (standard deviation, SD=0.0006) and 0.981 (SD=0.0058), respectively. The corresponding mean RMSE values were 98.72 t/km² and 274.07 t/km² (Figure 6(b)). Although the train-test performance gap suggests some degree of overfitting, the model effectively captured the nonlinear associations between carbon storage and its predictors. This finding also indicates the need for further predictor consolidation.

We subsequently calculated the mean importance of each predictor and estimated its 95% confidence interval (CI) using the bootstrap percentile method. As shown in Figure 7, NDVI and elevation together accounted for more than 92% of total feature importance, whereas the other eight predictors contributed less than 8%. Thus, the spatial variation in carbon storage across the PRD was primarily associated with vegetation and topographic characteristics, while socioeconomic variables had comparatively limited predictive importance. These results provide further support for streamlining the predictor set.



(a) Corss-validation analysis result



(c) Bootstrap iterations

Figure 6 Cross-validation and bootstrap iterations for ten predictors

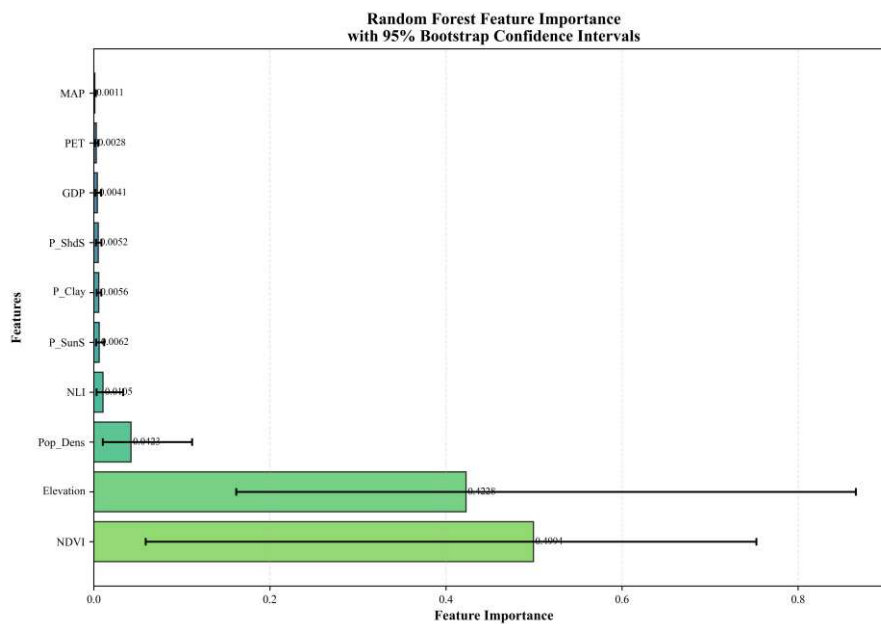


Figure 7 Feature importance analysis for ten predictors

3.3.3 Optimization of predictor variables and RFR models

Despite strong predictive and CV performance, the initial ten-predictor system showed limited efficiency. The eight least important variables contributed less than 8% of total feature importance, while the bootstrap CIs for MAP, PET, and GDP included or approached zero. Moreover, the higher test-set RMSE suggested some overfitting, indicating that weak or redundant predictors may have increased model complexity without improving generalizability.

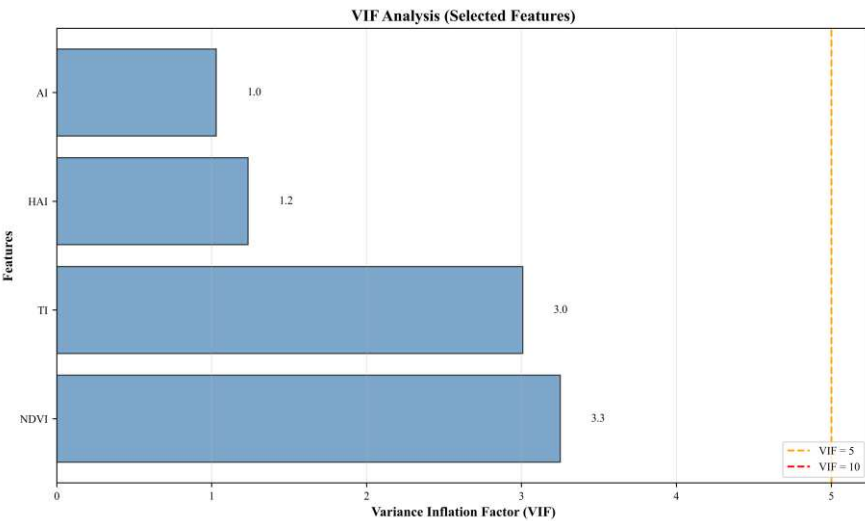
To address these issues, conceptually related variables were consolidated into composite indices. NDVI was retained because of its dominant contribution, whereas P_Clay was removed owing to its low feature importance (0.56%) and weak associations with variables from other dimensions. Elevation, P_SunS, and P_ShdS were integrated through PCA to construct a Topographic Index (TI). The KMO statistic was marginally acceptable (0.509), and Bartlett's test was significant ($p < 0.001$). The first component had an eigenvalue of 1.571 and explained 52.37% of the variance. Therefore, its scores were used to represent TI.

Pop_Dens, GDP, and NLI were similarly combined into a Human Activity Intensity index (HAI). PCA was supported by a KMO value of 0.707 and a significant Bartlett's test ($p < 0.001$). The first component explained 84.19% of the total variance, and all communalities exceeded 0.75 (Pop_Dens = 0.902, GDP = 0.863, and NLI = 0.761), revealing adequate representation of the original variables. MAP and PET were combined into an Aridity Index (AI), with higher values indicating drier conditions. The optimized system thus comprised four predictors, i.e., NDVI, TI, HAI, and AI, representing vegetation productivity, topographic constraints, anthropogenic disturbance, and climatic water availability, respectively.

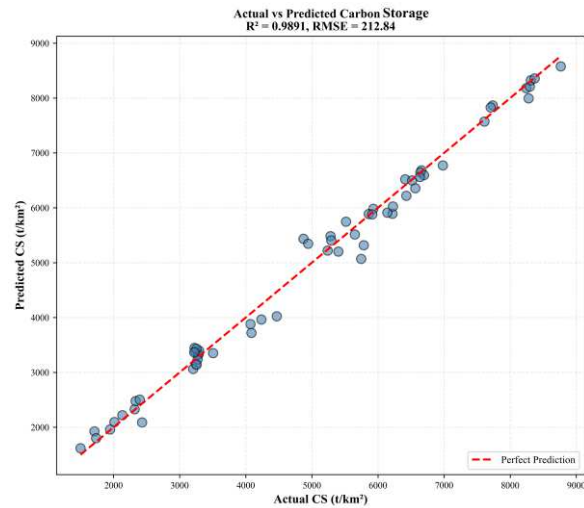
As shown in Figure 8(a), the optimized system exhibited low multicollinearity, with VIF values ranging from 1.0 to 3.3, all below the conservative threshold of 5. Predictive performance remained strong, with a test-set of 0.9891 (Figure 8(b)). The reduced difference between training- and test-set RMSE values (118.48 and 212.84 t km, respectively) also suggested modestly reduced overfitting. CV confirmed model robustness, yielding a mean of 0.9789 (SD=0.008).

The optimized RFR model was further evaluated using 5,000 bootstrap iterations. Compared with the original model, it exhibited a more concentrated R^2 distribution, lower variability, and no extreme outliers. The 95% bootstrap CIs for all four feature-importance estimates excluded zero, supporting the stability of the optimized predictor set (Figure 9(a)).

As shown in Figure 9(b), the relatively wide confidence interval for NDVI (0.10–0.79) may reflect shared information with TI, their combined contribution reached 94.9%, highlighting vegetation conditions and topographic setting as the primary correlates of spatial variation in carbon storage. HAI contributed 4.0% (95% CI: 0.021–0.085), indicating a stable but limited anthropogenic contribution, whereas AI accounted for only 1.1% (95% CI: 0.005–0.018), consistent with the PRD's predominantly humid climate. These results demonstrate the robustness of the optimized model and the dominant roles of vegetation and topography.

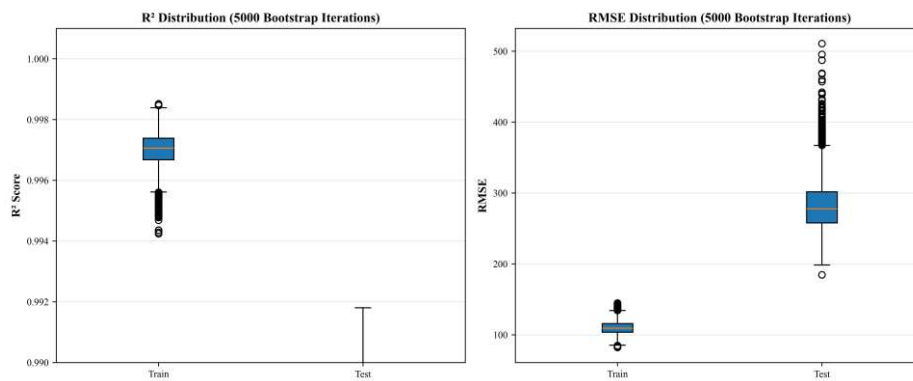


(a) VIF tests

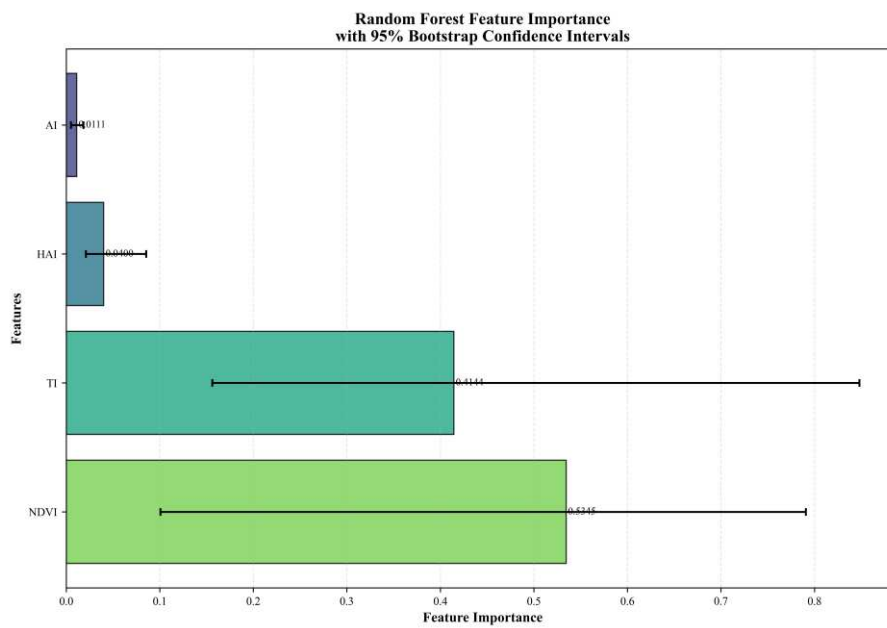


(b) Corss-validation

Figure 8 VIF tests and cross-validation analysis to the four predictors



(a) Bootstrap iterations



(b) Feature importance analysis

Figure 9 Bootstrap interanion and feature importance analysis to the four predictors

As shown in Figure 10, the PDPs revealed nonlinear associations between the four core predictors and predicted carbon storage. Predicted carbon storage increased sharply when NDVI exceeded approximately 0.5, while its association with TI strengthened initially before reaching a plateau. HAI exhibited a consistently negative association, whereas AI showed a weak and irregular pattern. These results underscore the greater predictive importance of vegetation and topography relative to anthropogenic activity and climatic aridity. The two-dimensional interaction plots (Figure 11) further demonstrated the joint effects of NDVI and TI. The highest predicted carbon storage (7,322.40 t/km²) occurred under high NDVI and low TI conditions, reflecting that well-vegetated areas with favorable topographic characteristics support greater carbon storage.

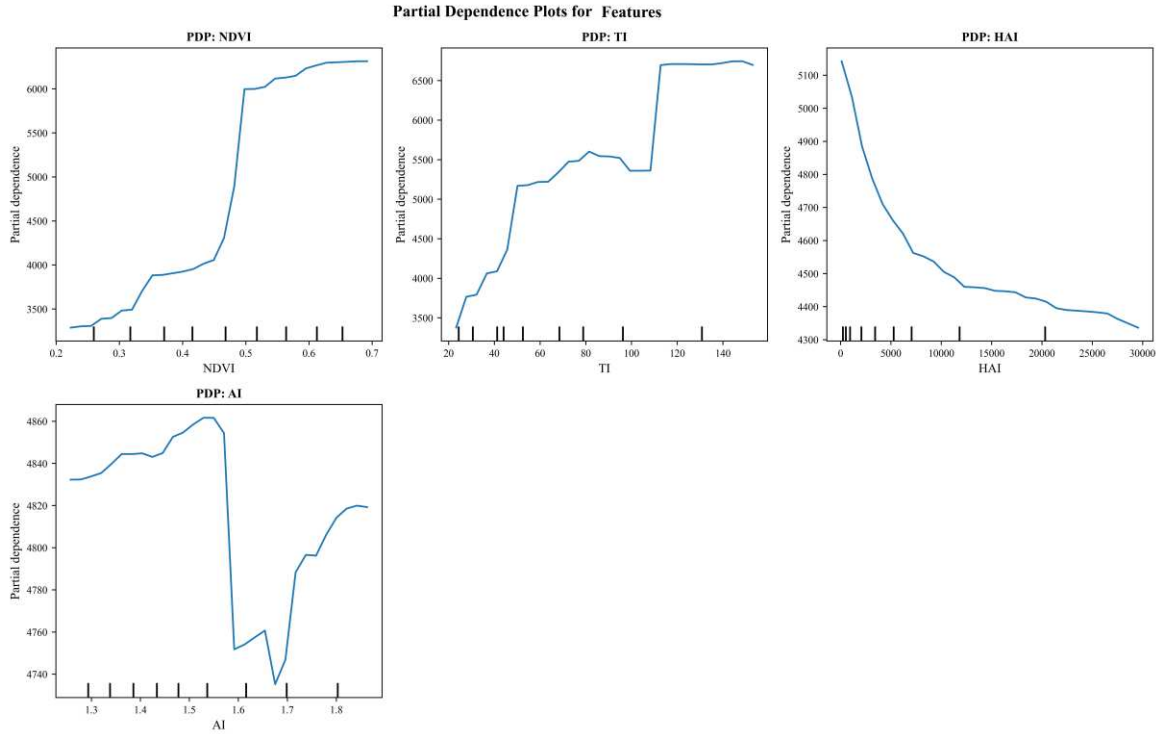


Figure 10 PDPs for the four core predictors

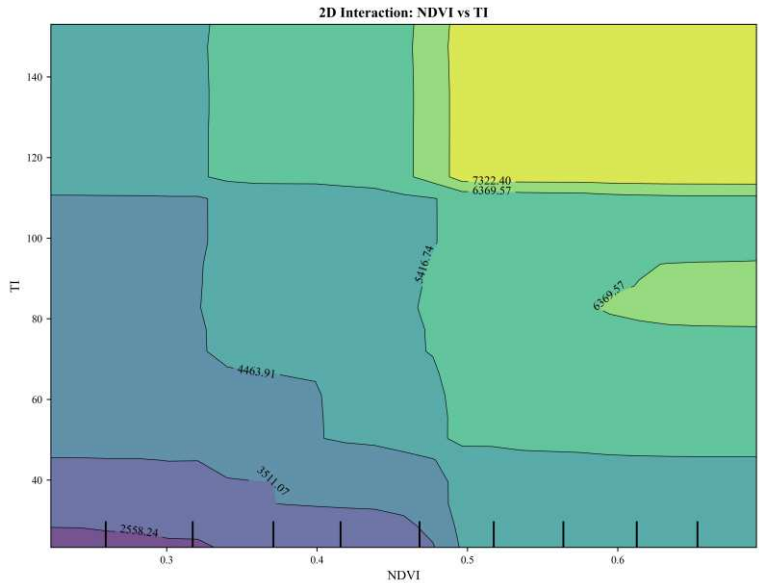


Figure 11 Synergistic effects between NDVI and TI

3.4 GTWR

To characterize spatiotemporal heterogeneity (2000-2023) in the drivers of carbon storage, we implemented a GTWR model in GWmodelS 2.0 using four core predictors, i.e., NDVI, TI, HAI, and AI. The model used district- and county-level units across the PRD, a Gaussian kernel, and an adaptive bandwidth of 20 nearest neighbors selected through CV. It demonstrated strong explanatory performance, with an $R^2=0.9729$ and an adjusted $R^2=0.9685$; the AIC and AICc values were 4,370.15 and 4,413.00, respectively. Local R^2 values exceeded 0.93 throughout the PRD and were highest in core urban areas and low-elevation plains (Figure 12), indicating consistently strong performance even in regions characterized by intensive human activity and complex land-use patterns.

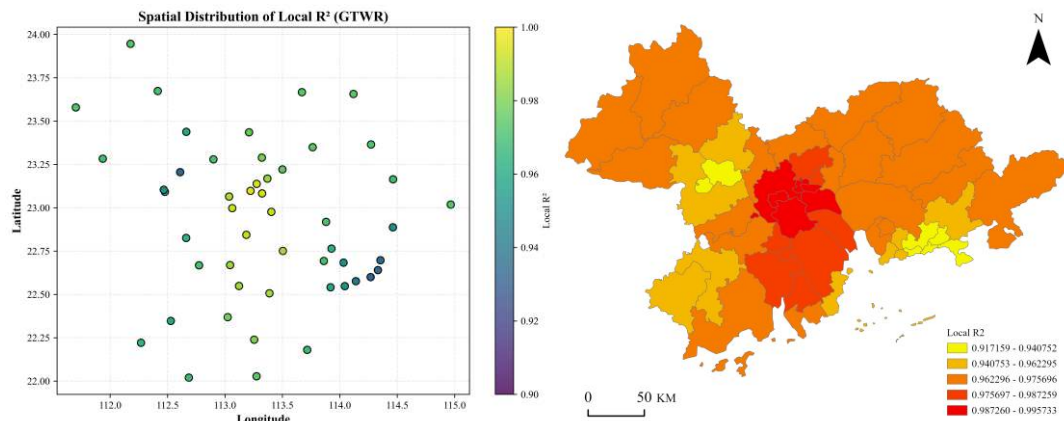


Figure 12 Spatial distribution of Local R^2 (GTWR)

3.4.1 Spatiotemporal evolution of GTWR coefficients

GTWR coefficients revealed substantial spatial nonstationarity in the relationships between the four core predictors and carbon storage. To compare local-effect magnitudes, predictor importance was quantified using the mean absolute value of the standardized coefficients (Figure 13). Kernel density estimation was then used to characterize the coefficient distributions for each predictor (Figure 14).

The intercept accounted for 10.5% of the modeled variation and may characterize unobserved differences in environmental conditions, land-use history, and policy contexts. Its spatial pattern exhibited west-east and peripheral-core gradients (Figure 15(a)). Positive values in western ecological areas suggest favorable baseline conditions for carbon storage, whereas negative values in eastern coastal areas may reflect intensive urban development. Near-zero values in the urban core may indicate offsetting effects of ecological degradation and conservation efforts.

NDVI had the highest standardized importance (81.9%), identifying vegetation condition as the dominant spatial correlate of carbon storage across the PRD. Its coefficient distribution was distinctly bimodal, yet coefficients were positive in all districts and counties. Values generally ranged from 4,000 to 9,000 t/km², with a mean of 6,299.13 t/km², indicating a consistently positive association. NDVI effects were strongest in the northern and western hilly regions and ecological conservation zones, where contiguous forests provide substantial carbon-sequestration capacity. They were weaker in urban cores and coastal plains, where habitat fragmentation likely constrains this function (Figure 15(b)). The absolute local t -values exceeded 1.96 throughout the study area, further supporting the statistical significance and spatial dominance of NDVI.

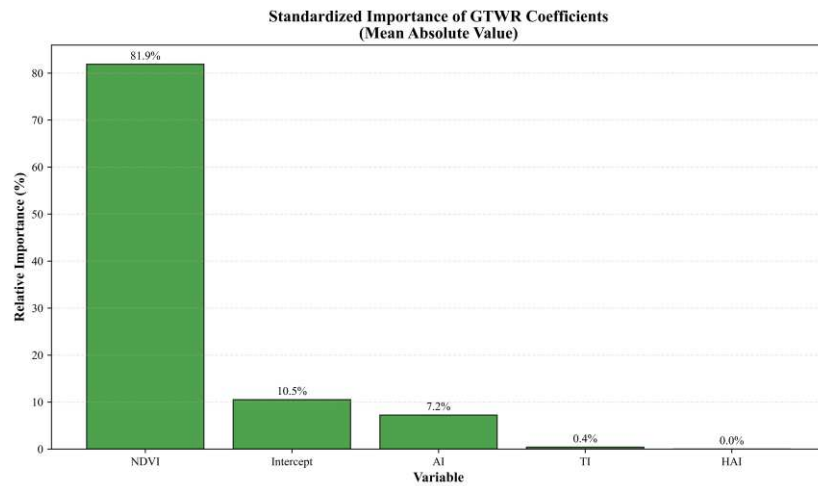


Figure 13 Standardized importance of GTWR coefficients

Kernel Density Estimation of GTWR Coefficients

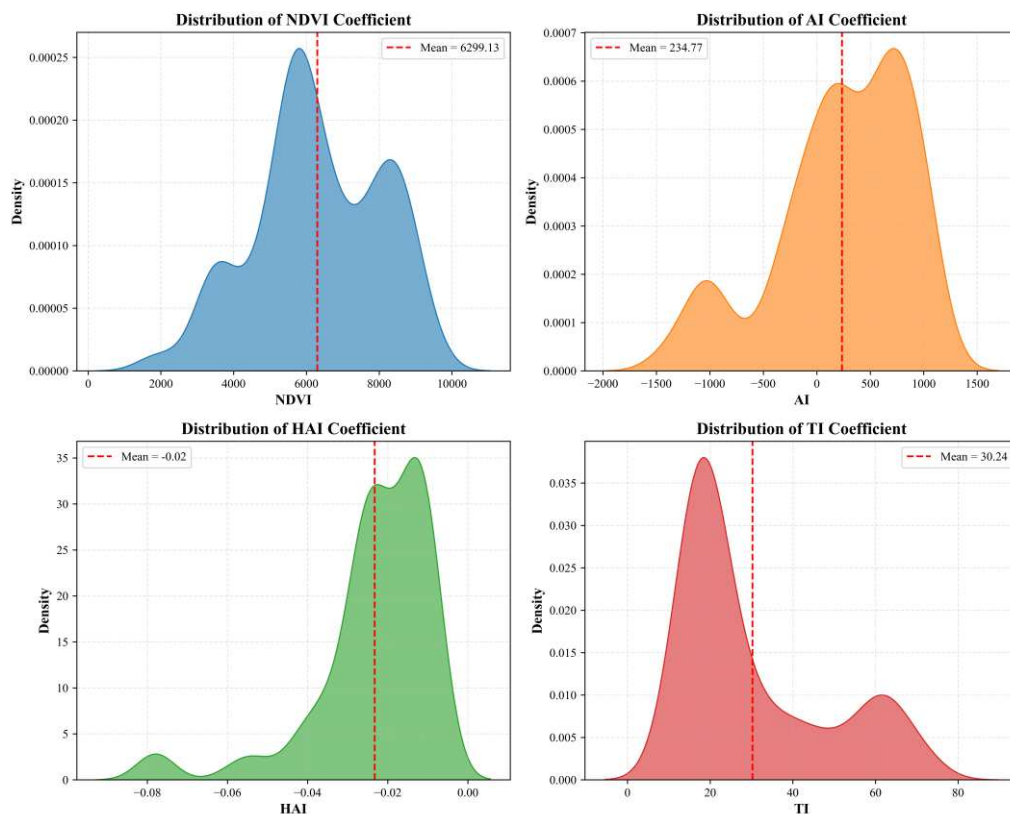


Figure 14 Kernel density estimations of GTWR coefficients

AI had the second-highest standardized importance, accounting for 7.2%. Its kernel density distribution was multimodal and extended across negative and positive values, with a positive mean coefficient of 234.77 t/km², indicating pronounced spatial heterogeneity. As shown in Figure 15(c), AI generally exerted negative effects in the eastern and northern PRD but positive effects in the western and southern coastal areas. This reversal in coefficient signs underscores the context dependence of the relationship between AI and carbon storage. Local coefficients were statistically significant in most districts and counties, further demonstrating that AI is an important local determinant of carbon storage.

TI and HAI made limited contributions at the regional scale, with standardized importance values of 0.4% and approximately 0%, respectively, but both exhibited significant spatially

localized effects. TI coefficients were consistently positive, and their bimodal kernel density distribution peaked at approximately 20 and 60 t/km², with a mean of 30.24 t/km². This pattern suggests a generally positive influence on carbon storage, particularly in the northern and western hilly areas, where moderate topographic variability may promote carbon accumulation. The effect was weaker in high-elevation mountainous areas and coastal plains (Figure 15(d)). In contrast, HAI coefficients were negative across all spatial units, indicating that human activity generally inhibited carbon storage. This effect was strongest in highly urbanized cities, including Guangzhou, Shenzhen, and Foshan, and weaker in ecological conservation and agricultural areas (Figure 15(e)). Thus, although TI and HAI had minimal regional importance, their local effects were pronounced.

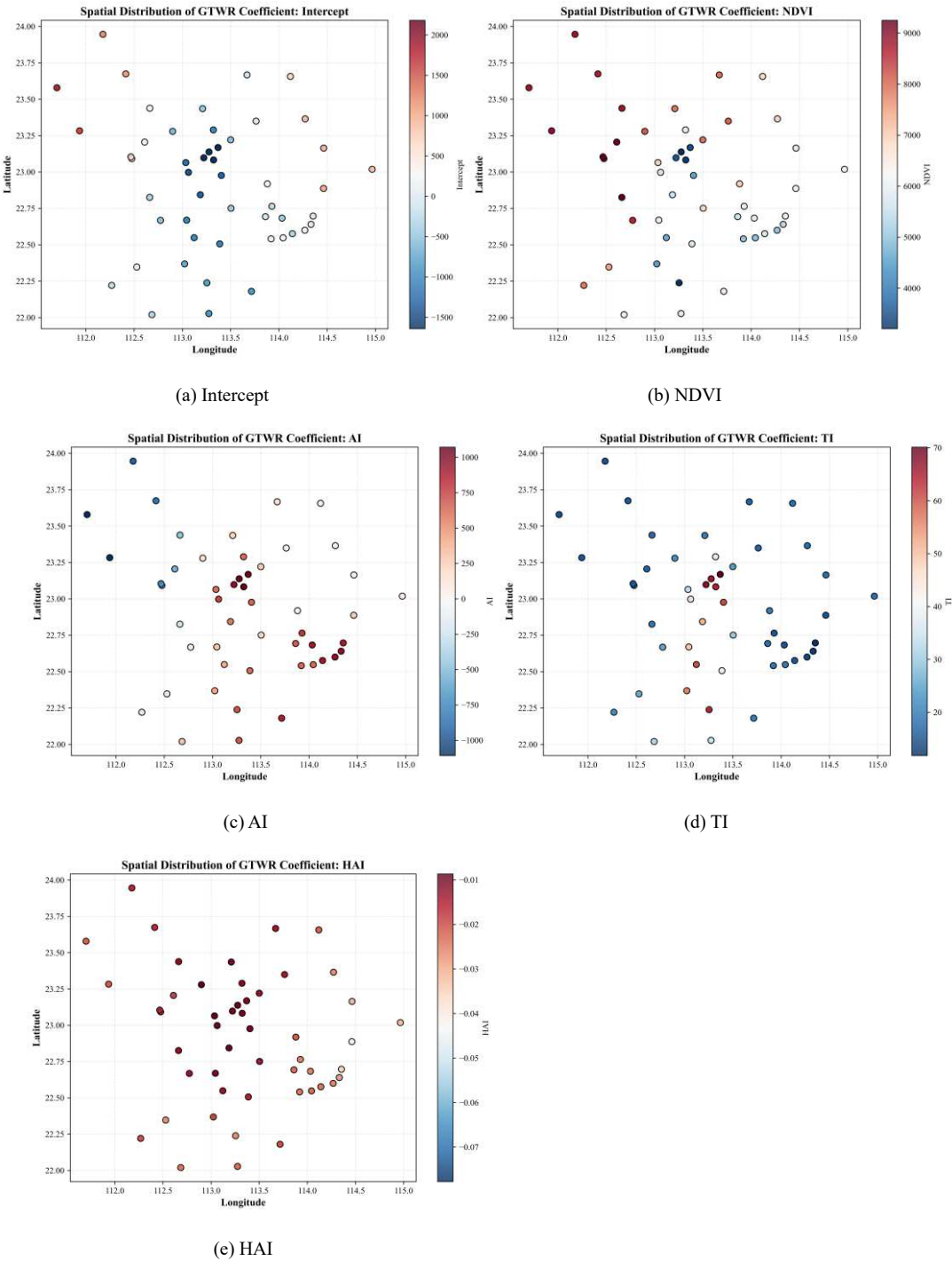


Figure 15 Spatial distribution patterns of GTWR coefficients

3.4.2 Synergistic and antagonistic interactions among four core predictors

To examine spatial covariation among the four core predictors, we constructed a matrix of their GTWR coefficients, integrating marginal distributions with pairwise associations. As shown in Figure 16, NDVI and TI coefficients were strongly positively correlated, indicating that their estimated effects varied concordantly across space. Conversely, the negative association between NDVI and HAI suggests spatial opposition between vegetation-mediated carbon sequestration and anthropogenic pressure. The relationship between NDVI and AI was stratified, reflecting spatial heterogeneity in the hydroclimatic regulation of vegetation effects. The clustering patterns involving TI, HAI, and AI further reveal differentiated spatial coupling among topographic, anthropogenic, and climatic influences.

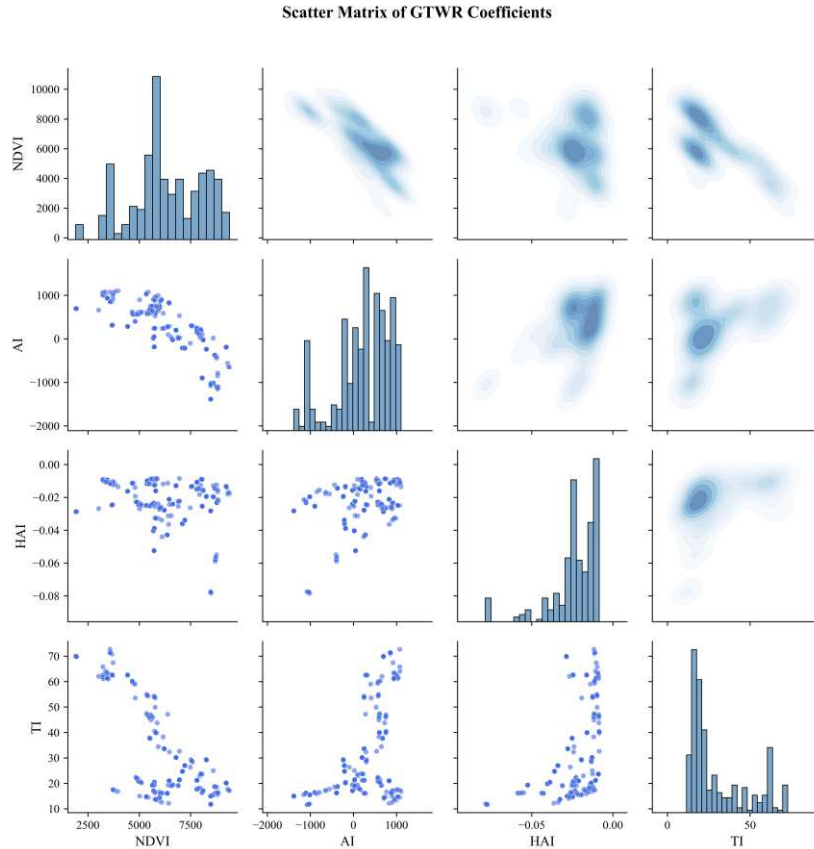


Figure 16 Scatterplot matrix of GTWR coefficients

3.5 XGBoost-SHAP

GTWR revealed substantial spatiotemporal heterogeneity in the drivers (predictors) of carbon storage across the PRD. To examine temporal variation in the predictive contributions of the four core variables, separate XGBoost models were developed for 2000, 2005, 2010, 2015, 2020, and 2023. Test set performance was assessed using R^2 and RMSE.

As reported in Table 9, model performance improved from 2000 and 2015 but deteriorated thereafter. Over this period, R^2 increased from 0.974 to 0.981, while RMSE declined to 304.4 t/km². By 2020 and 2023, R^2 had decreased to 0.951 and 0.946, respectively, whereas RMSE increased to 488.6 and 509.6 t/km². This decline may indicate that post-2015 changes, such as accelerated urbanization, land-cover transitions, and extreme climatic events, were not fully captured by the four predictors. Nevertheless, R^2 exceeded 0.94 in all study years, revealing consistently strong predictive performance.

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Table 9 Model performance metrics

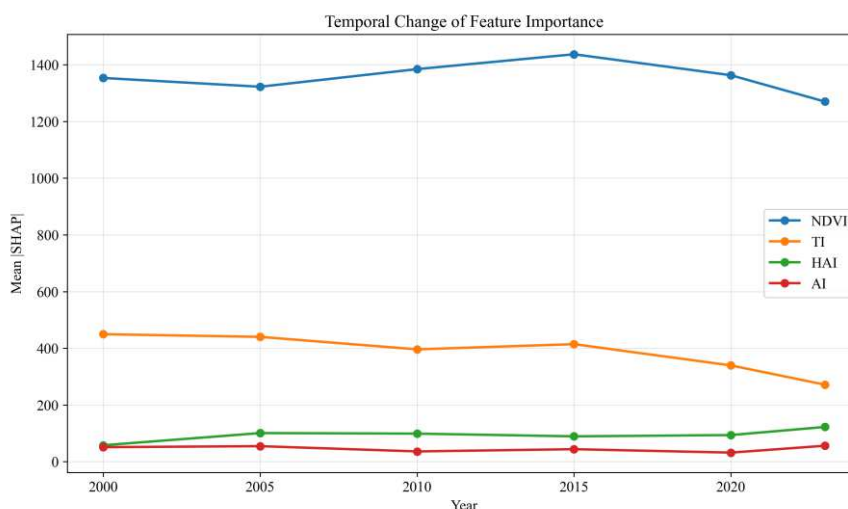
Year	R^2	RMSE (t/km ²)
2000	0.974	345.7
2005	0.957	453.7
2010	0.973	371.2
2015	0.981	304.4
2020	0.951	488.6
2023	0.946	509.6

549 3.5.1 Predictive contribution and evolution characteristics of variables

550 Table 10 reports the annual mean absolute SHAP values (Mean |SHAP|), which measure each
 551 core predictor's average contribution to model predictions, while Figure 17 depicts their temporal
 552 variation. NDVI consistently ranked as the most influential predictor, with Mean |SHAP| values of
 553 approximately 1,300–1,440 t/km². Its contribution peaked around 2015 before declining overall. TI
 554 remained the second most influential variable, although its Mean Mean |SHAP| decreased from
 555 approximately 450 t/km² in 2000 to 270 t/km² in 2023, indicating a diminishing contribution of
 556 topography to predictive performance. In contrast, HAI increased from approximately 60 to 120
 557 t/km², suggesting a growing role for human activity. AI consistently had the lowest and most
 558 stable contribution, with values ranging from approximately 30 to 60 t/km².

559 **Table 10 Feature importance (Mean |SHAP|) by year**

Year	NDVI (t/km ²)	TI (t/km ²)	HAI (t/km ²)	AI (t/km ²)
2000	1353.26	449.55	57.86	51.20
2005	1322.38	440.14	100.86	54.68
2010	1384.46	396.12	98.97	36.17
2015	1436.89	414.45	89.32	44.06
2020	1362.89	339.51	93.84	32.00
2023	1269.86	271.48	122.51	56.26



560

561

Figure 17 Temporal evolutions of annual mean absolute SHAP values

Figure 18 presents the normalized SHAP importance of the predictor variables, highlighting their relative contributions to carbon-storage predictions and their temporal variation. NDVI consistently accounted for more than 70% of the total importance, confirming vegetation condition as the primary predictor of spatial variation in carbon storage. Although its Mean |SHAP| peaked around 2015, its absolute contribution reached a local maximum around 2020, indicating a distinction between relative importance and contribution magnitude. In contrast, the relative importance of TI generally declined, whereas that of HAI increased gradually. This shift suggests that the predictive structure evolved from being dominated by vegetation and topographic conditions toward a more integrated influence of natural and anthropogenic factors. AI maintained a low and relatively stable contribution share of approximately 1%-3%. Above results revealed that vegetation remained the dominant predictor, while topographic importance decreased and anthropogenic importance increased, complementing the spatial heterogeneity identified by GTWR.

Accordingly, the study period can be divided into two phases based on XGBoost performance and predictor importance. During the relatively stable phase (2000-2015), model performance improved steadily, with NDVI and TI remaining the dominant predictors. This pattern coincided with sustained ecological protection and vegetation restoration in the PRD. During the transition phase (2015-2023), model performance declined as the importance of HAI increased, suggesting a stronger association between human activity and spatial variation in carbon storage. These changes coincided with accelerated urban expansion and transport-infrastructure development, which may have intensified forest fragmentation in hilly areas and contributed to the conversion of cropland and other ecological land in the plains. However, absolute SHAP values indicate contribution magnitude rather than effect direction. The direction and nonlinear characteristics of HAI effects therefore require further assessment using SHAP dependence plots.

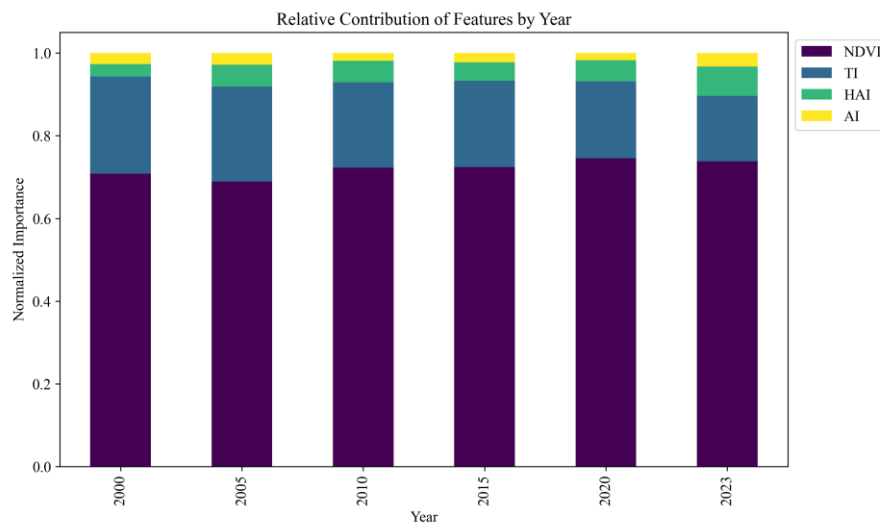


Figure 18 Standardized relative contribution evolution of four predictors

3.5.2 Nonlinear driver effects based on SHAP dependence patterns

To examine nonlinear relationships between the predictors and carbon-storage predictions, SHAP summary and PDPs were generated for 2000, 2005, 2010, 2015, 2020, and 2023. Figure 19 summarizes the temporal patterns of the four core predictors. Positive and negative SHAP values indicate that a predictor increases or decreases a model prediction relative to the baseline, respectively, while their absolute magnitude represents contribution strength. NDVI exhibited a consistently positive but nonlinear association with predicted carbon storage, whereas HAI was generally negatively associated. TI also showed a nonlinear relationship, i.e., higher values were typically associated with positive SHAP values, although this contribution weakened over time. AI values were concentrated near zero, indicating limited incremental predictive information; their greater dispersion in some years nevertheless suggests modest temporal variation in its modeled association with carbon storage.

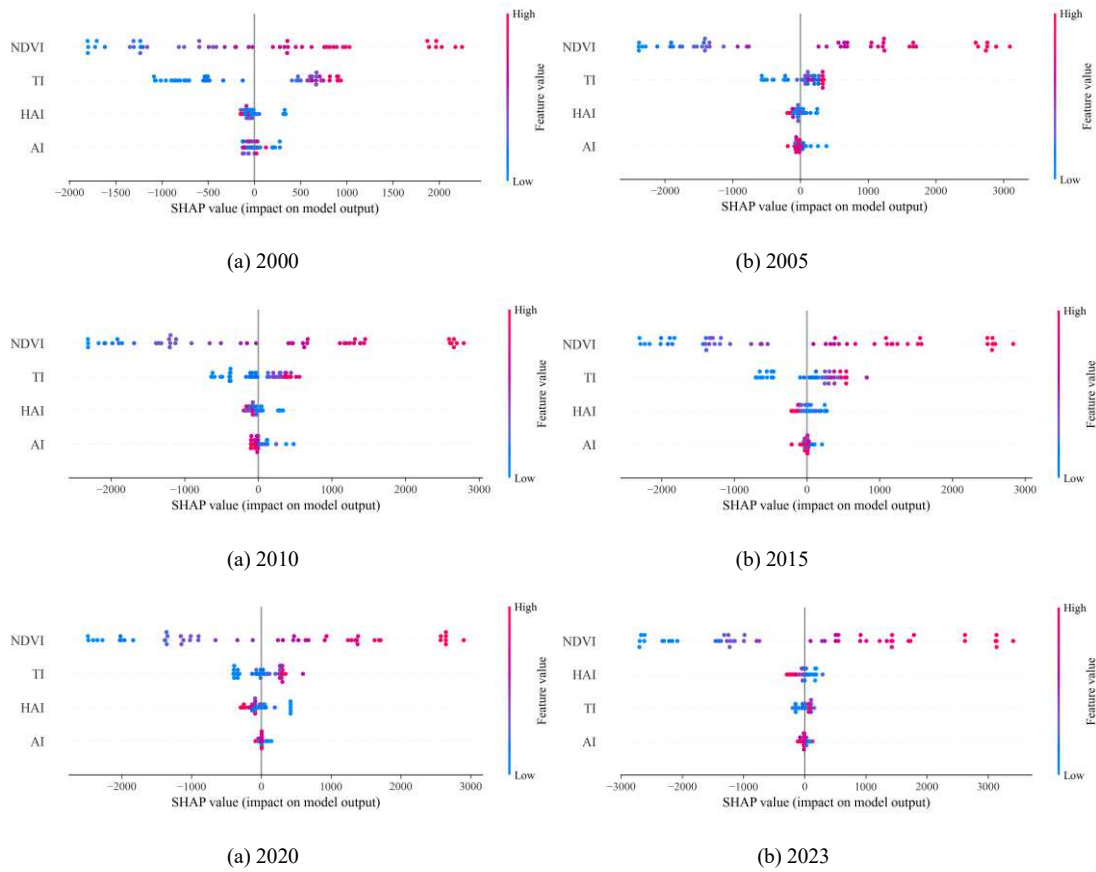


Figure 19 Temporal variations in SHAP dependence patterns from 2000-2023

Figure 20 presents annual SHAP dependence plots, highlighting temporal variation in the shape, range, and dispersion of predictor effects on carbon-storage estimates. The LOWESS curves characterize these nonlinear relationships, i.e., SHAP values above zero indicate predictions above the model baseline, whereas negative values indicate lower predictions.

NDVI exhibited a stable, monotonic positive association with predicted carbon storage (Figure 20(a)). Its SHAP values formed an S-shaped curve, i.e., they remained negative below approximately 0.48, increased rapidly between 0.50 and 0.60, and plateaued above 0.60. This pattern suggests that vegetation improvement may generate the largest marginal gains at intermediate NDVI levels, with diminishing gains under high vegetation cover. Positive SHAP values at high NDVI increased until 2015 but declined slightly thereafter, possibly reflecting intensified land-use and urbanization pressures.

TI was also positively associated with predicted carbon storage, although its contribution weakened markedly over time (Figure 20(b)). At high TI values, positive SHAP values approached 1,000 t/km² in 2000 but were only marginally above zero in 2023. Because topographic conditions change little over short periods, this decline likely reflects changes in their relative predictive importance rather than a reduction in their underlying ecological influence. Differences in land-cover patterns, predictor interactions, and annual sample composition may also have contributed.

HAI generally showed a negative association with predicted carbon storage, with increasingly negative contributions over time (Figure 20(c)). The LOWESS curves were relatively flat at low HAI values but changed sharply as HAI approached approximately 2,000, suggesting a nonlinear threshold beyond which intensified human activity was associated with substantially lower predicted carbon storage.

AI made a limited contribution, with most SHAP values concentrated near zero (Figure 20(b)). Although its effect range expanded in some years, indicating modest temporal or spatial variation, its low importance may reflect limited spatial variability in drought conditions across the PRD rather than the ecological irrelevance of hydrothermal conditions to carbon cycling.

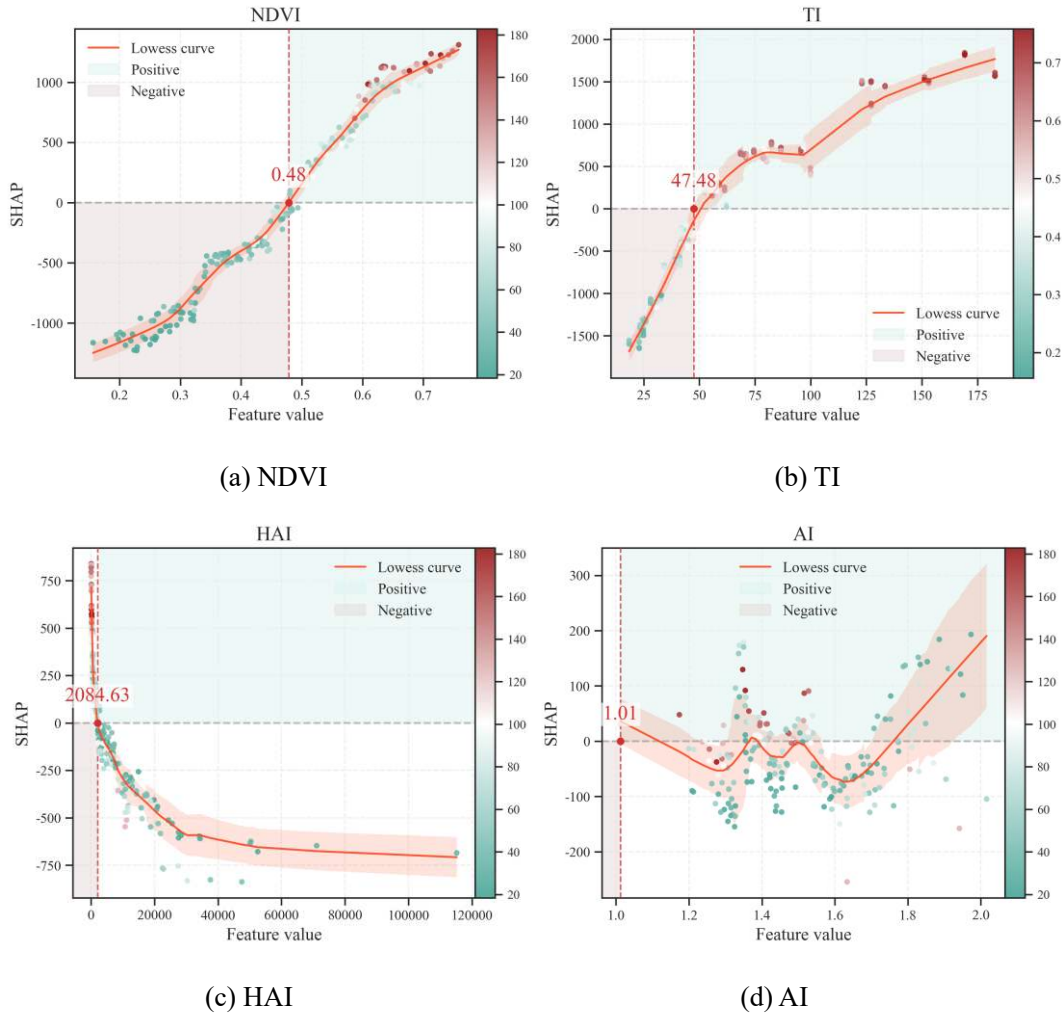


Figure 20 SHAP dependence patterns of the four predictors

4. Discussion

4.1 Integration of local heterogeneity and global contributions

This study integrates GTWR and XGBoost-SHAP to assess carbon-storage drivers in the PRD from complementary perspectives. GTWR characterizes spatial and temporal variations in the direction and magnitude of local effects, whereas XGBoost-SHAP quantifies global nonlinear contributions. Their integration provides a comprehensive interpretation of carbon-storage dynamics than either method alone. This framework effectively addresses the inability of a single modelling method, whether spatial regression (Zeng and Sun 2024; Guo et al. 2026) or machine learning (Ye et al. 2025), to simultaneously capture spatiotemporal nonstationarity and complex nonlinear interactions.

4.2 Stabilizing and marginal effects of NDVI

Both GTWR and XGBoost-SHAP identified NDVI as the strongest and most consistently positive predictor of carbon storage in the PRD, underscoring the importance of vegetation cover amid intensifying anthropogenic pressure. Its nonlinear SHAP response indicates that vegetation enhancement may yield the greatest marginal benefits in areas with low to moderate NDVI, whereas highly vegetated areas should prioritize conservation to preserve ecological integrity and carbon-storage capacity. Consistent with findings from other urban agglomerations in southern China (Zhang et al. 2025; Cao et al. 2023), these results confirm the dominant role of vegetation condition in shaping carbon-storage capacity.

4.3 Declining topographic influence

The declining TI importance and GTWR coefficient magnitudes indicate a weakening influence of topography on carbon storage. In 2000, mountainous areas such as Conghua, Longmen, and Enping exhibited relatively high carbon storage, likely because rugged terrain constrained development and preserved extensive, contiguous forests. By 2023, however, GTWR coefficients had declined across many high-TI areas, coinciding with expanded tourism, transport infrastructure, and understory economic activities. This pattern suggests that topographic constraints alone may be insufficient to safeguard long-term carbon storage. Whereas previous studies have generally treated terrain as a static constraint on human disturbance (Guo et al. 2026; Li and Li 2025), this study provides empirical evidence that diversified human activities may progressively weaken this protective effect.

4.4 Increasing anthropogenic pressure and nonlinear effects

The growing explanatory of HAI, alongside its progressively negative SHAP values, suggests that anthropogenic effects have expanded from localized land conversion to broader regional pressure. During 2000-2023, the marginal carbon penalty associated with high HAI intensified markedly, consistent with the compounding effects of urban expansion, industrial agglomeration, and population growth. The SHAP dependence plots further reveal a potential breakpoint beyond which carbon-storage reductions accelerate. Although this breakpoint requires independent validation before being treated as a management threshold, it provides a basis for developing carbon-storage carrying-capacity indicators. Existing urban-carbon studies frequently adopt linear assumptions about human disturbance impacts (Wang et al. 2026; Sui et al. 2026). The detected nonlinear threshold effect in this work delivers more targeted support for differentiated territorial regulation.

4.5 Factor interaction and spatiotemporal coupling

Carbon-storage dynamics reflect the interplay between environmental conditions and human activities. The positive spatial correlation between the GTWR coefficients for NDVI and TI indicates that their local effects tend to coincide, while the SHAP interaction analysis suggests that TI moderates the contribution of NDVI. Specifically, the positive association between NDVI and carbon storage was stronger in high-TI areas than in lowland plains, possibly because rugged terrain constrains development, preserves vegetation continuity, and sustains favorable local environmental conditions. By contrast, the increasingly negative effect of HAI suggests intensifying anthropogenic disturbance. Previous attribution studies have largely focused on independent effects and paid limited attention to how topography may condition vegetation-related carbon sequestration (Wei et al. 2025; Liu et al. 2019; Zhou et al. 2024a). By integrating GTWR with XGBoost-SHAP analysis, this study provides a comprehensive assessment of these interactions and advances understanding of the hierarchical drivers of terrestrial carbon storage in megaregions.

4.6 Policy implications

Carbon-storage management in the PRD should move beyond expanding green-space area toward integrated governance combining ecosystem protection, development regulation, and vegetation-quality improvement. First, high-carbon mountainous and hilly areas should be protected through strict ecological zoning and controls on tourism, infrastructure, and dispersed construction. Second, highly urbanized areas should mitigate carbon-storage losses through urban forests, wetland restoration, ecological corridors, and context-appropriate vertical greening. Third, areas with low to moderate NDVI (approximately 0.3-0.6) should be prioritized for vegetation restoration, degraded-forest rehabilitation, and farmland ecological enhancement, where marginal carbon-stock gains are likely to be greatest.

5. Conclusion

This study integrates InVEST-based carbon-storage estimation, robust indicator screening, GTWR, and XGBoost-SHAP analysis to investigate carbon-storage dynamics in the PRD urban agglomeration from 2000 to 2023. The results indicate that these dynamics arise from the interacting effects of vegetation, topography, and human activity rather than from land-use change alone. NDVI was the strongest and most stable positive predictor, highlighting the importance of vegetation cover and quality. By contrast, the declining influence of TI suggests that topographic constraints have become less effective in safeguarding carbon storage. HAI exhibited an increasingly negative and nonlinear effect, indicating intensifying anthropogenic pressure and a potential threshold beyond which carbon-storage losses may accelerate, whereas AI made a comparatively weak and temporally stable contribution. The positive NDVI-TI interaction further suggests that topographic conditions enhance the contribution of vegetation in mountainous areas. Overall, the dominant mechanism has shifted from terrain-mediated vegetation protection toward a more complex regime characterized by persistent vegetation support, weakening topographic constraints, and intensifying human disturbance. Carbon-storage governance should therefore extend beyond green-space expansion toward integrated and spatially differentiated management. Key priorities include protecting high-carbon mountainous areas, controlling development intensity in urban cores, restoring areas with low to moderate vegetation cover, and developing early-warning indicators of anthropogenic pressure. These findings support differentiated strategies for carbon management, ecological restoration, and low-carbon spatial planning in the rapidly urbanizing PRD, while offering methodological insights for carbon-cycle research in comparable megacity regions worldwide.

This study integrates spatiotemporal heterogeneity analysis, nonlinear effect identification, and spatially differentiated governance to provide a transferable framework for carbon-storage management in rapidly urbanizing regions. However, three limitations remain. First, the lagged and cumulative effects of LUCC were not explicitly quantified. Second, InVEST estimates rely on literature-derived carbon-density parameters and therefore may not capture within-class spatial variability. Third, the district- and county-level analysis may obscure fine-scale processes and cross-scale interactions. Future research should address these limitations through dynamic LUCC modeling, locally calibrated carbon-density data, and multiscale analytical approaches.

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Author contribution statement

H.Z. and S.C wrote the main manuscript text. H.Z. and S.C reviewed and edited the main manuscript text. M.F. implemented the data analysis and prepared figures 1-7. All authors have read and agreed to the published version of the manuscript.

Data availability statement

All raw raster datasets can be accessed at <https://www.resdc.cn> and <https://data.tpdc.ac.cn/home> after free registration. All intermediate data, refined data, code, scripts, and analytical results used to support the findings of this study are available from the corresponding author upon request.

Ethical Approval and Informed Consent

Ethical Approval: This article does not contain any studies with human participants performed by any of the authors.

Informed Consent: This article does not contain any studies with human participants performed by any of the authors.

Conflicts of interest statement

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

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