



Role of urban green space structure and configuration in regulating land surface temperature in NCT Delhi using explainable artificial intelligence

Manish Kumar^a, Sourav Bhadwal^a, Netrananda Sahu^{b,*}

^a Department of Geography, School of Basic Sciences, Central university of Haryana, Jant-Pali, Mahendragarh, Haryana 123031, India

^b Department of Geography, Delhi School of Economics, University of Delhi, New Delhi 110007, India

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ABSTRACT

Urbanization-driven heat intensification poses a serious challenge to environmental sustainability and thermal comfort in megacities such as National Capital Territory (NCT) Delhi. The influence of green space structure and configuration on Land Surface Temperature (LST) remains under-explored. This study presents a novel framework that integrates Fragstats-derived green space metrics and explainable artificial intelligence (XAI) to assess the spatio-temporal impact of green space structure and configuration on LST in NCT Delhi. The LST and nine green space metrics were derived using the Landsat-8 (OLI/TIRS) imagery. Three machine and deep learning models i. e., Gradient Boosting Machine (GBM), Distributed Random Forest (DRF), and Deep Learning (DL) were developed to regress and predict LST using H2O AutoML package in Rstudio environment. Among these, GBM produced the highest predictive accuracy ($R^2 = 0.8859$) and was therefore selected for further interpretation using XAI techniques such as SHapley Additive exPlanations (SHAP) and Individual Conditional Expectation (ICE) plots. Results show that fragmented green spaces intensify surface heating, while cohesive and well-connected green space corridors promote cooling through enhanced evapotranspiration and shading. The findings highlight that not only the amount but also the spatial configuration of vegetation determines its cooling efficiency. Areas in East Delhi (Shahdara, Seelampur) and North-West Delhi (Narela, Bawana, Rohini Extension), characterized by high fragmentation, experience higher temperatures, whereas contiguous green space corridors of Central and South Delhi exhibit stronger cooling benefits. These insights provide actionable guidance for urban planners and policymakers to prioritize cohesive green space development in future urban planning for climate adaptation and mitigation.

1. Introduction

Rapid urbanization has led to substantial transformations in earth surface characteristics. The widespread conversion of natural and semi-natural areas into built-up landscapes, covered by asphalt and concrete, increases heat absorption and retention (Li et al., 2023; Mohajerani et al., 2017; Shaw et al., 2020). This leads to a consistently higher Land Surface Temperature (LST) in urban areas compared to their rural counterparts (Peng et al., 2018). Land use and land cover (LULC) change, which captures the dynamics of

* Corresponding author.

E-mail addresses: manish.ks@cuh.ac.in (M. Kumar), nsahu@geography.du.ac.in (N. Sahu).

urban expansion, serves as a key driver in understanding the changing LST characteristics of the urban regions. Rapid urban growth leads to fragmentation of green spaces, weakening their cooling functions like shading, evapotranspiration, and soil moisture regulation (Cheung et al., 2022; Pereira et al., 2024). Along with increasing LST, green space loss and fragmentation also degrades vital environmental services like air purification, carbon storage, and the ability to withstand extreme heat conditions (Munang et al., 2013; Pandey and Ghosh, 2023; N. Singh et al., 2020). Previous studies have shown that the expansion and improved spatial connectivity of urban green spaces play a crucial role in mitigating LST, particularly in rapidly urbanizing environments (Yang et al., 2017). Therefore, protecting and integrating well-designed green spaces into urban planning is essential for improving environmental quality and reducing LST extremes in rapidly expanding cities.

In recent decades, the global urban population has expanded from 751 million in 1950 to 4.2 billion in 2018, with Asia contributing the highest proportion (54 %), followed by Africa (13 %) and others (World Urbanization Prospects, 2019). The expansion is expected to continue, with projections indicating an increase in the global urbanization rate from 56.2 % in 2020 to 60.4 % by 2030 (World Urbanization Prospects, 2022). India mirrors global urbanization trends. With its urban population growing from 78.94 million in 1961 to 377.10 million in 2011, the country experienced a significant 378 % increase (Census, 2011). By 2030, it is projected that 40.76 % of the country's population will reside in urban areas (United Nations Population Fund, 2007). Within India, National Capital Territory (NCT) Delhi is one of the fastest growing, complex urban regions (Biswas and Gangwar, 2021). It is presently ranked as the world's second-largest urban agglomeration with a population exceeding 29 million. By 2027, NCT Delhi is projected to surpass Tokyo to become the most populous city in the world (Kleer and Nawrot, 2018; Sarkar and Lakshmana, 2024). The rapid urban growth in NCT Delhi has led to serious environmental issues, particularly a stronger Urban Heat Island (UHI) effect, where city areas exhibit higher LST compared to nearby rural regions. Various empirical studies have highlighted the increasing intensity of UHI phenomenon in NCT Delhi. N. Yadav and Sharma, 2018 reported a temperature difference of 6–7 °C between central urban zones and adjacent rural areas during peak summer, largely attributed to dense built-up surfaces and vegetation loss. Similarly, Mallick et al., 2013 found that commercial districts with minimal green cover exhibited 4 °C higher LST than suburban green zones, underscoring the need for climate-responsive urban planning.

Over the past few decades, the integration of spatial analysis and environmental modelling has advanced the understanding urban LST dynamics (Huo et al., 2021; Mustafa et al., 2021; Reinert et al., 2023). Early studies primarily relied on statistical techniques such as Ordinary Least Squares, spatial regression, and Geographically Weighted Regression (Kalota, 2017; Kashki et al., 2021). While these methods created foundational insights, they offer limited application in capturing nonlinear interactions and struggle with high-dimensional data, that is typical in spatial ecological models (W. Zhang et al., 2024). Recent research has demonstrated that machine learning (ML) models can effectively quantify the cooling influence of urban green spaces on LST, revealing the critical role of vegetation morphology and spatial configuration in regulating urban heat (Lin et al., 2023). In parallel, ML techniques such as Support Vector Machines (SVM), Random Forest (RF), etc. have shown superior performance in urban heat and climate studies by accommodating complex relationships and improving predictive accuracy (Cheng et al., 2025; Mathew et al., 2019; Q. Wang et al., 2022). However, most of these approaches depend on manual tuning, algorithm selection, and subjective parameterization, which can introduce bias and hinder reproducibility. To address these limitations, the present study leverages Automated Machine Learning (AutoML) via the H2O platform, enabling automated model selection and hyperparameter optimization through a consistent, unbiased, and scalable workflow (Azevedo et al., 2024; Haberl and Thalmann, 2025; R. Sharma and Patel, 2024). In the AutoML framework, three high-performing algorithms Gradient Boosting Machine (GBM), Distributed Random Forest (DRF), and Deep Learning (DL) were selected based on their predictive strength and prior validation in geospatial and climatological research. The selected models represent diverse algorithmic paradigms that capture bias-variance trade-offs in different ways. Collectively these models span a continuum from interpretable ensembles (GBM and DRF) to higher efficiency architectures (DL). This allows for a balanced evaluation of predictive strength and generalization behaviour. GBM is widely recognized for its efficiency in structured data and its robustness in modelling nonlinear environmental processes (C. Chen et al., 2024). DRF offers excellent generalizability and stability across large, complex datasets (Z. Wang et al., 2024), while DL architectures are increasingly applied to spatial modelling due to their ability to capture hierarchical feature relationships (Ahmed et al., 2023). This study incorporates Explainable Artificial Intelligence (XAI) techniques to address a key limitation of machine learning (ML) models. Although the selected algorithms (GBM, DRF, and DL) are powerful tools for regressing relationships between green space metrics and LST, they inherently function as black-box models (Majid et al., 2025; Zednik, 2021). This means that they provide high predictive accuracy but offer limited transparency regarding the relative contribution, direction, and interaction of predictor variables. Such opacity restricts their usefulness for ecological interpretation, where understanding the underlying mechanisms is as important as achieving robust predictions. To overcome this disadvantage, XAI techniques were integrated to make the ML models more interpretable. Specifically, Shapley Additive Explanations (SHAP) and Individual Conditional Expectation (ICE) plots to capture global feature importance and local response patterns. SHAP quantifies how much each predictor contributes to the overall model output, while ICE illustrates how changes in a variable influence the predicted. The integrated approach was selected over alternative XAI techniques (e.g., Local Interpretable Model-Agnostic Explanations, Partial Dependence Plot, etc.) due to its stability, interpretability, and robustness in modelling complex nonlinear interactions along with thresholding effects typical of urban thermal systems (Chen et al., 2025). By integrating ML with XAI, the study moves beyond purely predictive modelling and provides detailed insights regarding the role of green space structure in moderating urban temperatures. This integration strengthens the ecological relevance of the findings and supports more informed decision-making for urban planning and climate resilience. It reveals the patterns that are not accessible through standalone ML implementation, such as how fragmentation, patch cohesion, or vegetation continuity influence LST under varying conditions. Furthermore, XAI techniques have gained substantial popularity in air-quality and hydrological research (Hao et al., 2024; Yang et al., 2022). However, their application in urban thermal landscape modelling remains limited. This study also addresses the methodological gap by implementing XAI in the context of a

rapidly urbanizing region of NCT Delhi, thereby extending its relevance to urban heat mitigation research.

A comprehensive investigation into the dynamics of UHI phenomenon and mitigating role of urban green spaces becomes imperative for promoting climate resilience and sustainable urban planning (Gupta and De, 2025). Grounded in the principles of landscape ecology and urban climatology (Forman and Godron, 1986; Oke, 1982), this study conceptualizes vegetation structure as a key spatial regulator of surface energy balance and urban thermal environment. Vegetation, as a vital ecosystem service, mitigates thermal stress through various mechanisms such as evapotranspiration, shading, and surface albedo modification (Bolund and Hunhammar, 1999; Oke, 1989). However, many previous studies in this direction often prioritized vegetation extent metrics (e.g., Normalized Difference Vegetation Index or NDVI) while neglecting spatial structure and configuration, which are critical for understanding the thermal function of green spaces within urban systems. Spatially integrated, model-driven research that captures the complexities of UHI phenomenon in light of green space structure and configuration remains scarce. Consequently, there is a pressing need for spatially integrated, model-based research that accounts for the complex interactions between UHI intensity and the structural characteristics of urban greenery, a domain that remains largely underexplored. Addressing this gap, the present study introduces a scientifically grounded, scalable framework that links vegetation landscape structure to LST patterns using XAI techniques, offering both predictive power and interpretability for urban climate resilience planning. The primary objective of this study is to model and interpret the relationships between urban green space structure and LST in NCT Delhi using integrated ML-XAI approach. Furthermore, by linking high-resolution spatial metrics with state-of-the-art predictive and interpretive modelling, the study advances a replicable and policy-relevant methodology for understanding and mitigating urban heat. This framework not only contributes to the academic discourse on urban thermal environments but also offers practical insights for designing climate-resilient, vegetation-informed urban planning strategies.

2. Materials and methods

The methodological framework to assess the role of urban green space in regulating LST in the NCT Delhi in this study is presented in Fig. 2.

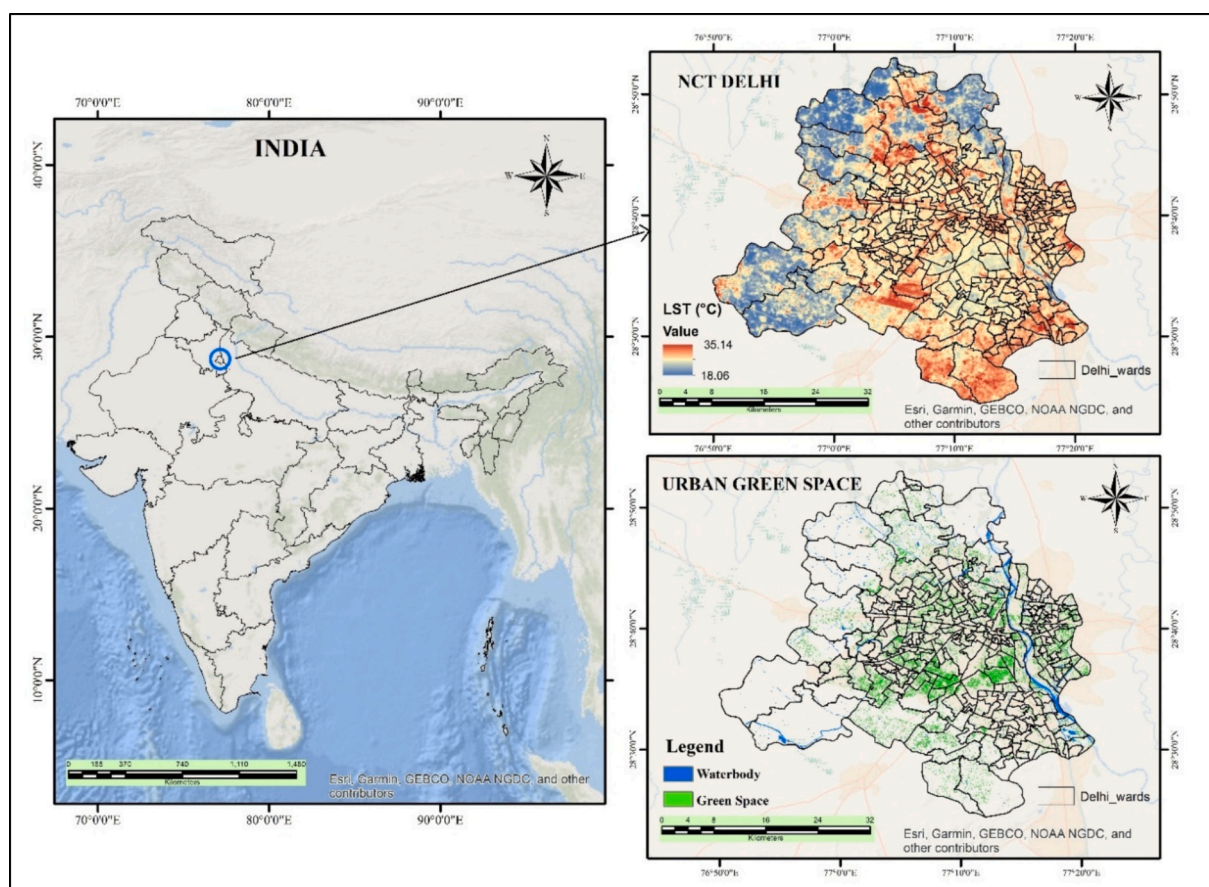


Fig. 2. Methodological flow diagram.

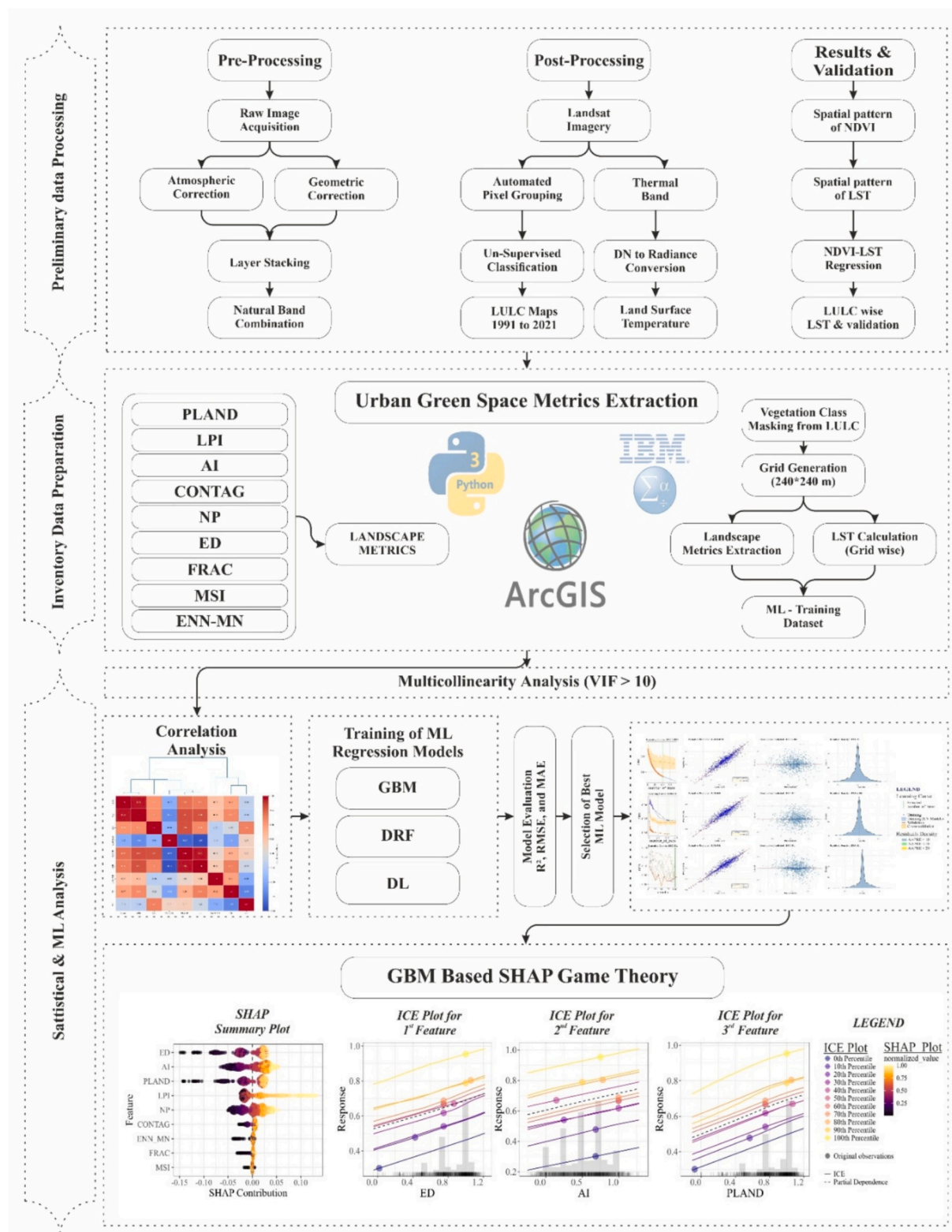


Fig. 1. Location map of the study area.

2.1. Study area

NCT Delhi, situated in northern India, covers an area of 1484 km² and lies between 28°24' to 28°53' N latitudes and 76°50' to 77°20' E longitudes (Fig. 1). It shares borders with the states of Haryana on three sides and Uttar Pradesh to the east. As the political and administrative capital of India, NCT Delhi has undergone intense urbanization over the last few decades, making it one of the most densely populated metropolitan regions in the country (M. Sharma and Abhay, 2022, Majid et al., 2024). This rapid transformation has significantly altered the city's land use patterns, with substantial expansion of built-up areas and a corresponding decline in natural and semi-natural land covers (Bhadwal and Kumar, 2025). However, amidst this urban sprawl, NCT Delhi continues to retain critical green infrastructure. It includes the Ridge Forest (part of the ancient Aravalli range), Sanjay Van, Nehru Park, Lodhi Gardens, and extensive institutional green belts, particularly in South and Central Delhi. Geographically, the city exhibits limited terrain variability, primarily comprising the Plain regions, the Yamuna Flood Plain, and the Delhi Ridge (Majid et al., 2024). The Yamuna River, flowing along the eastern boundary, further influences the city's ecological zones and microclimates.

NCT Delhi is situated at an average elevation of 216 m above sea level and has a semi-arid climate (Köppen: BSh) characterized by extreme seasonal variations. Summers are particularly harsh, with mean monthly temperatures reaching 34.5 °C and maximums exceeding 45 °C in peak summer months of May and June. Winters are cold and dry, with minimum temperatures dropping to 3 to 5 °C during December and January (Manikandan et al., 2019). NCT Delhi receives an average annual rainfall of 714 mm. Nearly 75 % of the precipitation occurs during the monsoon period from July to September (Mushtaq et al., 2024). These climatic extremes contribute to significant temporal and spatial variations in LST. In recent years, NCT Delhi has shown clear signs of UHI effects, with LST values rising more sharply in densely built-up zones compared to vegetated and forested areas (P. Singh et al., 2022). The variation in LST across NCT Delhi is influenced by the distribution and size of urban green spaces. This spatial contrast highlights the city's significance as a case study for understanding the role of green infrastructure in shaping urban thermal environments. NCT Delhi's diverse landscape, which includes dense urban areas as well as scattered green patches, offers a suitable context to examine how urban green space affects LST over time.

2.2. Data collection & pre-processing

This study utilized multi-temporal Landsat satellite imagery from 1991, 2001, 2011, and 2021 to analyse the relationship between urban green space and LST in NCT Delhi. Thermal and optical data were acquired from Landsat 5 and 8 sensors through the United States Geological Survey (USGS) Earth Explorer (<https://earthexplorer.usgs.gov>). To ensure seasonal consistency across the years, imagery corresponding to the pre-monsoon period (March–April) was acquired, representing the early summer phase when LST begin to rise sharply (Saha et al., 2023). NDVI maps were generated to evaluate vegetation dynamics and their relationship with LST, while unsupervised classification was performed to derive six LULC classes for each study year. To assess the spatial characteristics of green areas, nine vegetation-specific landscape metrics were extracted using FRAGSTATS within a standardized fishnet grid framework. All data processing was conducted using ArcGIS 10.8, and FRAGSTATS, forming the basis for the analytical framework presented in the following subsections.

2.2.1. Landsat thermal and optical imagery

To assess LST and vegetation cover over time, this study utilized thermal and optical bands from multi-temporal Landsat satellite imagery for the years 1991, 2001, 2011, and 2021. The imagery was sourced from USGS Earth Explorer and included data from Landsat 5 Thematic Mapper (TM) and Landsat 8 Operational Land Imager/Thermal Infrared Sensor (OLI/TIRS). Satellite images were selected from the months of March and April, a period that marks the onset of the regions' pre-monsoon summer. This timing was deliberately chosen to capture rising LST before the occurrence of convective rainfall and atmospheric disturbances typical of May–June (Sinha et al., 2019). It also ensures temporal consistency in vegetation and surface conditions across years. All selected images met a cloud cover threshold of less than 10 %, ensuring optimal surface visibility and data quality for temperature and vegetation analysis. The optical bands used for NDVI computation were acquired at a 30-m spatial resolution, whereas the thermal bands originally at 120 m for Landsat 5 TM and 100 m for Landsat 8 were resampled to 30 m to ensure spatial consistency during pixel-wise analysis (Table 1) (Garg and Salunke, 2024). All datasets were geometrically corrected and projected to the WGS 84 / UTM Zone 43 N coordinate system. Standard radiometric calibration and atmospheric correction procedures were applied prior to the retrieval of

Table 1

Acquisition dates and parameters of Landsat thermal and optical imagery used for LST and NDVI estimation.

Acquisition date	Satellite	Sensor	Bands Used	Purpose	Resolution (m)	Local Time (GMT + 5:30)
1991	Landsat-5	TM	Band 6 (Thermal), Bands 3,4 (Optical)	LST, NDVI	120 (Thermal), 30 (Optical)	10:25 AM
2001	Landsat-5	TM	Band 6 (Thermal), Bands 3,4 (Optical)	LST, NDVI	120 (Thermal), 30 (Optical)	10:24 AM
2011	Landsat-5	TM	Band 6 (Thermal), Bands 3,4 (Optical)	LST, NDVI	120 (Thermal), 30 (Optical)	10:26 AM
2021	Landsat-8	OLI / TIRS	Band 10 (Thermal), Bands 4,5 (Optical)	LST, NDVI	100 (Thermal), 30 (Optical)	10:23 AM

LST. LST estimation followed a multi-step process, including conversion of digital numbers to radiance, calculation of brightness temperature, assignment of emissivity based on NDVI thresholds, and final transformation to LST values in degrees Celsius. In addition, NDVI was determined using the red and near-infrared bands for each year to assess vegetation density and distribution. These NDVI layers were later used to examine the inverse relationship between green space and LST across time, forming a critical component of the analytical framework.

2.2.2. LULC classification and accuracy assessment

LULC classification formed a foundational step in this study, as it enabled the precise delineation of vegetation areas required for the extraction of green space landscape metrics. Multi-temporal Landsat images from 1991, 2001, 2011, and 2021 were classified using the ISODATA unsupervised algorithm to produce consistent LULC maps. This approach was chosen because reliable ground-truth data were not available for all time periods, which limited the use of supervised methods. ISODATA automatically groups pixels with similar spectral characteristics and iteratively adjusts class boundaries to reduce within-class variance and improve separation between land-cover types (Lemenkova, 2021). This adaptive process ensures accurate classification in heterogeneous urban and vegetated environments such as those found in the NCT of Delhi. The classified outputs were interpreted and categorized into six major land cover classes that is waterbody, vegetation, forest, agriculture, built-up, and barren land. NDVI layers were used in conjunction to assist in distinguishing vegetation-based classes and to reduce confusion between spectrally similar classes such as built-up and barren land. Visual validation of the classified outputs was carried out using high-resolution historical imagery from Google Earth to support the accurate assignment of class labels and enhance thematic consistency. Finally, the LULC maps (1991, 2001, 2011, and 2021) were validated using 500 stratified random points for each year. The reference data were derived from Google Earth imagery for 1991, 2001, and 2011, and from ground-truth observations collected in 2021. The LULC maps demonstrated high classification accuracy, as confirmed by the computed accuracy and Kappa statistics. The classification accuracies for the years 1991, 2001, 2011, and 2021 were recorded as 91.00 %, 88.18 %, 86.73 %, and 93.09 %, respectively, indicating acceptable classification performance across the temporal span, with the highest accuracy achieved in the most recent year (Bhadwal and Kumar, 2025). Importantly, the classified vegetation class served as the basis for the extraction of landscape configuration metrics, which were calculated exclusively on vegetation patches. These metrics were later used to analyse their spatial and statistical relationship with LST. Thus, the LULC classification not only captured urban expansion trends but also directly supported the study's core objective of quantifying how green space structure influences urban thermal patterns.

2.3. Land surface temperature (LST) retrieval

A single-channel method was used to retrieve the LST (Duan et al., 2019; Jiménez-Muñoz and Sobrino, 2003; Käfer et al., 2020). Band 6 of Landsat-5 TM was used to estimate LST, while for Landsat-8 OLI/TIRS, Band 10 was utilized for the same purpose. The procedure of retrieval can be summarized in four steps:

Calculation of Spectral radiance (Chander et al., 2009).

$$L_{\lambda} = \left(\frac{L_{max} - L_{min}}{QCAL_{max} - QCAL_{min}} \right) \times (QCAL - QCAL_{min}) + L_{min} \quad (1)$$

Where:

L_{λ} = Spectral radiance at the top of the atmosphere.

$QCAL$ = Quantized and calibrated standard product pixel values (DN).

$QCAL_{min}$ = Minimum quantized and calibrated standard product pixel value (DN).

$QCAL_{max}$ = Maximum quantized and calibrated standard product pixel value (DN).

L_{max} = Spectral radiance scaled to $QCAL_{max}$ ($W.m^{-2}.Sr^{-1}.\mu m^{-1}$).

L_{min} = Spectral radiance scaled to $QCAL_{min}$ ($W.m^{-2}.Sr^{-1}.\mu m^{-1}$).

Emissivity: Estimating land surface emissivity (ϵ) is a critical step in retrieving LST, as ϵ serves as a scaling factor that adjusts blackbody radiation (as described by Planck's law) to reflect the actual thermal energy emitted by the Earth's surface. It essentially represents the surface's efficiency in radiating thermal energy into the atmosphere. To accurately determine emissivity, it is first necessary to compute the NDVI (Sobrino and Raissouni, 2000).

$$NDVI = \left(\frac{NIR - RED}{NIR + RED} \right) \quad (2)$$

Where:

NIR = near infrared band value of a pixel (band 4 for Landsat 5 and band 5 for Landsat 8).

RED = red band value of the same pixel (band 3 for Landsat 5 and band 4 for Landsat 8).

Emissivity (ϵ):

for $NDVI < 0$ (it is classified as water) then $\epsilon = 0.991$.

$0 < NDVI < 0.2$ (it is classified as bare soil) then $\epsilon = 0.966$.

$0.2 < NDVI < 0.5$ (mixed of soil and vegetation cover – Sparse vegetation) then $\epsilon = \text{eq. (3)}$

$NDVI > 0.5$ (it is classified as vegetation) then $\epsilon = 0.973$.

Following (Alexander, 2020).

$$\varepsilon = m \times P_v + n \quad (3)$$

where: P_v = Proportion of vegetation, $m = 0.004$ and $n = 0.986$ (F. Wang et al., 2015).

$$P_v = \left(\frac{NDVI - NDVI_{min}}{NDVI - NDVI_{max}} \right)^2 \quad (4)$$

where:

$NDVI_{min}$ = Minimum NDVI value.

$NDVI_{max}$ = Maximum NDVI value.

Atmospheric correction: In the third step, L_λ was corrected for atmospheric effect using the procedure proposed by (Avdan and Jovanovska, 2016; Markham and Barker, 1985). This correction approach was selected because it forms the radiative transfer foundation of the Single Channel algorithm, providing a physically based and computationally efficient means of adjusting at-sensor radiance for atmospheric transmittance and path radiance using a single thermal band. The required atmospheric parameters were extracted directly from the scene-specific metadata (.MTL) files accompanying each Landsat 5 TM and Landsat 8 OLI/TIRS image, which provides all necessary calibration and radiometric rescaling coefficients for accurate scene-based atmospheric correction across acquisition dates.

$$L_C = \frac{L_\lambda - L_\mu - \tau(1 - \varepsilon)L_d}{\tau\varepsilon} \quad (5)$$

where:

L_C = radiance of a blackbody target by kinetic temperature.

L_λ = spectral radiance at the top of the atmosphere.

L_μ = upwelling radiance.

τ = atmospheric transmission.

ε = emissivity.

L_d = downwelling radiance.

Calculation of LST in Celsius (F. Wang et al., 2015)

$$LST = \frac{K_2}{\ln\left(\frac{K_1}{K_2} + 1\right)} - 273.15 \quad (6)$$

where: K_1 = Band- specific calibration constant in $W/m^2 \text{ sr } \mu m$ from the metadata (Table 2).

K_2 = Band- specific calibration constant in Kelvin from the metadata (Table 2).

2.4. Urban green space metrics extraction

To quantify the spatial configuration of urban green space and assess its potential influence on LST, this study focused exclusively on the vegetation class identified in the classified LULC map of 2021. A uniform fishnet grid of 240×240 m was generated and applied only to the spatial extent of vegetated areas. This targeted approach ensured that the analysis remained thematically focused by excluding non-vegetated zones such as built-up, water, and barren land. The chosen grid size corresponded to the 30-m resolution of Landsat imagery, encompassing 64 pixels (8×8) per grid cell sufficient to capture local spatial variability while maintaining a robust number of samples for statistical analysis and ML-XAI modelling. This intermediate scale also minimizes scale sensitivity in the computation of landscape metrics, as finer grids tend to introduce spatial noise while coarser grids dilute local heterogeneity. Similar resolutions (~ 210 – 240 m) have been shown to yield stable relationships between land-cover configuration and LST in previous multi-scale analyses (Lu et al., 2020; Terfa et al., 2020). This scale also ensures a sufficient number of analytical units for reliable ML model training (Tisseyre et al., 2018). The extraction of vegetation-based spatial metrics within each grid was automated using a Python script executed in Jupyter Notebook, addressing the limitations of manual processing given the scale of data (Bosch, 2019). This procedure resulted in a structured dataset comprising landscape metric values for each vegetated grid cell, which served as input for subsequent statistical analysis linking vegetation structure to LST patterns.

2.5. Landscape metrics analysis

A total of nine class-level landscape metrics were computed to characterize the spatial properties of urban green space for the year

Table 2
Thermal band calibration constant for specific Landsat satellites.

Satellite	Band	K_1	K_2
Landsat-8 OLI/TIRS	Band 10	774.8853	1321.0789
Landsat-5 TM	Band 6	607.76	1260.56

2021 (Table 3). The 2021 vegetation grid was selected as it provides the most recent and spatially reliable representation of green-space configuration, ensuring robust quantification of patch structure, dominance, and connectivity. These metrics were derived from the vegetation-specific grid dataset prepared in the previous step and calculated using Python-based workflow to ensure consistency, efficiency, and reproducibility. This spatially explicit analytical framework aligns with recent geospatial assessments demonstrating that optimizing the spatial configuration of urban green spaces can substantially enhance city-level thermal comfort (Gupta and De, 2024).

PLAND (Percentage of Landscape) quantified the proportion of each grid cell covered by vegetation, serving as a direct indicator of green space abundance. LPI (Largest Patch Index) captured the dominance of the largest contiguous vegetation patch, often linked to ecological resilience and thermal regulation potential. AI (Aggregation Index) measured the degree of spatial clustering among vegetation patches, while CONTAG (Contagion Index) described the overall continuity or dispersion of vegetated areas across each grid (A. Chen et al., 2014a).

To evaluate fragmentation, NP (Number of Patches) indicated the count of discrete vegetation clusters, and ED (Edge Density) expressed the perimeter length of patches relative to grid area, suggesting edge effects and patch exposure. Shape complexity was assessed through FRAC (Fractal Dimension Index), reflecting the geometric irregularity of patches, and MSI (Mean Shape Index), which calculated the average deviation from standard patch forms. Lastly, ENN-MN (Euclidean Nearest Neighbour - Mean Distance) measured average distances between vegetation patches, offering insight into spatial isolation and structural connectivity (Asgarian et al., 2015; Y. Liu et al., 2018; Zhou et al., 2011). These metrics collectively served as explanatory variables in analyzing the relationship between urban vegetation structure and LST, thereby supporting a deeper understanding of how spatial patterns of green space contribute to urban thermal dynamics.

2.6. Statistical and machine learning analysis

To evaluate the influence of urban green space on LST, an ML-XAI modelling framework was developed using the nine-landscape metrics derived from vegetation grids as predictor variables. As a prerequisite to model construction, a two-step diagnostic was conducted to assess inter-variable relationships and eliminate potential redundancies among predictors. First, a correlation analysis was performed to examine pairwise relationships among the nine-landscape metrics using Pearson's correlation coefficient. This step was intended to identify strong linear associations that could lead to redundancy in ML-XAI modelling (Kumar and Chong, 2018). Next, multicollinearity was assessed through the computation of the Variance Inflation Factor (VIF). Variables exhibiting high multicollinearity ($VIF > 5$ or 10) were considered for exclusion from the modelling process to enhance model stability and interpretability (Kim, 2019; Mahmood, 2024). This feature refinement step ensured that the selected predictor variables contributed unique, non-overlapping information to the regression models.

Following this data preparation, the modelling was implemented using the AutoML module of the H2O in the R software environment (LeDell and Poirier, 2020). AutoML is a framework that automates end-to-end process of model development, including data preprocessing, feature selection, algorithm selection, hyperparameter optimization, and model validation. It systematically assesses multiple ML regression models and parameter combinations to identify the most accurate predictive model for a given dataset, minimizing manual intervention and bias in model development (Omar et al., 2023). From the AutoML leaderboard, three high-performing algorithms GBM, DRF, and DL were selected for detailed analysis. These models were implemented to capture varying degrees of model complexity and bias-variance characteristics. Hyperparameter tuning employed random grid search with 10-fold

Table 3

Description and formulas of Landscape Metrics used in the study.

Landscape Metric	Abbreviation	Formula	Description	Units	Range
Percent of landscape	PLAND	$PLAND = (A_i / A) \times 100$	Proportion of total area occupied by a particular patch type; indicates landscape composition and dominance.	Percent	$0 < PLAND \leq 100$
Largest patch index	LPI	$LPI = (\max(A_i) / A) \times 100$	Percentage of total landscape area comprised by the largest patch; reflects spatial dominance of the largest patch.	Percent	$0 < LPI \leq 100$
Aggregation index	AI	$AI = (g_i / \max(g_i)) \times 100$	Measures the degree of aggregation of patches; calculated from adjacencies among pixels of the same class.	Percent	$0 \leq AI \leq 100$
Contagion index	CONTAG	$CONTAG = -\sum (P_{ij} * \ln(P_{ij}))$	Indicates the level of clumping or dispersion of patch types across the landscape; considers class adjacency and proportion.	Percent	$0 \leq CONTAG \leq 100$
Number of patches	NP	NP = total patch count	Total count of discrete patches of a particular class within the landscape.	None	$NP \geq 1$
Edge density	ED	$ED = (E / A) \times 10,000$	Sum of the lengths of all edge segments involving the patch type, divided by total landscape area.	m/ha	$ED > 0$
Fractal dimension index	FRAC	$FRAC = 2 \times \ln(0.25 \times P) / \ln(a)$	Quantifies patch shape complexity; higher values indicate more irregular patch shapes.	None	$1 \leq FRAC \leq 2$
Mean shape index	MSI	$MSI = \sum [P_i / (2\sqrt{\pi A_i})] / n$	Mean shape index across all patches; compares patch shapes to standard geometries.	None	$MSI \geq 1$
Euclidean nearest neighbour (mean)	ENN-MN	ENN-MN = mean (distance)	Average distance to the nearest neighboring patch of the same class, based on patch centroids.	Meters	$ENN-MN \geq 0$

Note: A = Total landscape area; A_i = Area of class i; $\max(A_i)$ = Area of the largest patch; g_i = Number of like adjacencies for class i; $\max(g_i)$ = Maximum possible adjacencies for class i; P = Patch perimeter; a = Patch area; P_i = Perimeter of patch i; A_i = Area of patch i; n = Number of patches; distance = Distance to the nearest patch of the same class; P_{ij} = Probability that a cell of class i is adjacent to class j.

cross-validation and early-stopping criteria (stopping_rounds = 5, stopping_metric = RMSE, and stopping_tolerance = 0.001). The best model from each algorithm family was selected based on the lowest cross-validated RMSE and subsequently validated using an independent hold-out test set.

The ML regression models were trained using the final set of landscape metrics to predict LST values across the study area with parameterization as discussed above. The dataset was divided into a training set and an external hold-out test set. Model performance was evaluated using a suite of statistical indicators including the R^2 , RMSE, and MAE (Karunasingha, 2022; Tatachar, 2021; W. Wang and Lu, 2018). This performance evaluation helps in identifying the best performing ML regression model. These ML regression models operate as *black-box* models, yielding limited transparency regarding why particular variables influence the output and how they interact within the model. Therefore, XAI techniques (SHAP and ICE) were integrated with the best performing model to interpret model behaviour, assess the relative influence of each predictor, and understand the sensitivity of LST to changes in the predictors (Nohara et al., 2022). SHAP provides a unified framework for estimating the marginal contribution of each feature to the model's prediction, both globally and at the individual instance level (Covert et al., 2020). It operates on the principle of cooperative game theory where the predictions of an ML regression model are considered as outcomes of a game and the predictor variables (landscape metrics, in the present study) act as the players (Majid et al., 2025). Following the procedure given in Majid et al., 2025, the SHAP values were calculated for each feature as the difference between the predictions made by the baseline model (including the complete set of independent variables) and the new models (involving independent features excluding the one for which the SHAP is to be determined). The determined SHAP values of the landscape metrics reflect their feature importance in influencing the LST. ICE plots, another visualization-based technique explains how the LST (dependent variable) depends on and varies with the landscape metrics (independent variables) (Molnar, 2024). It depicts the changes in the model predictions with changes in a single predictor holding all other features constant.

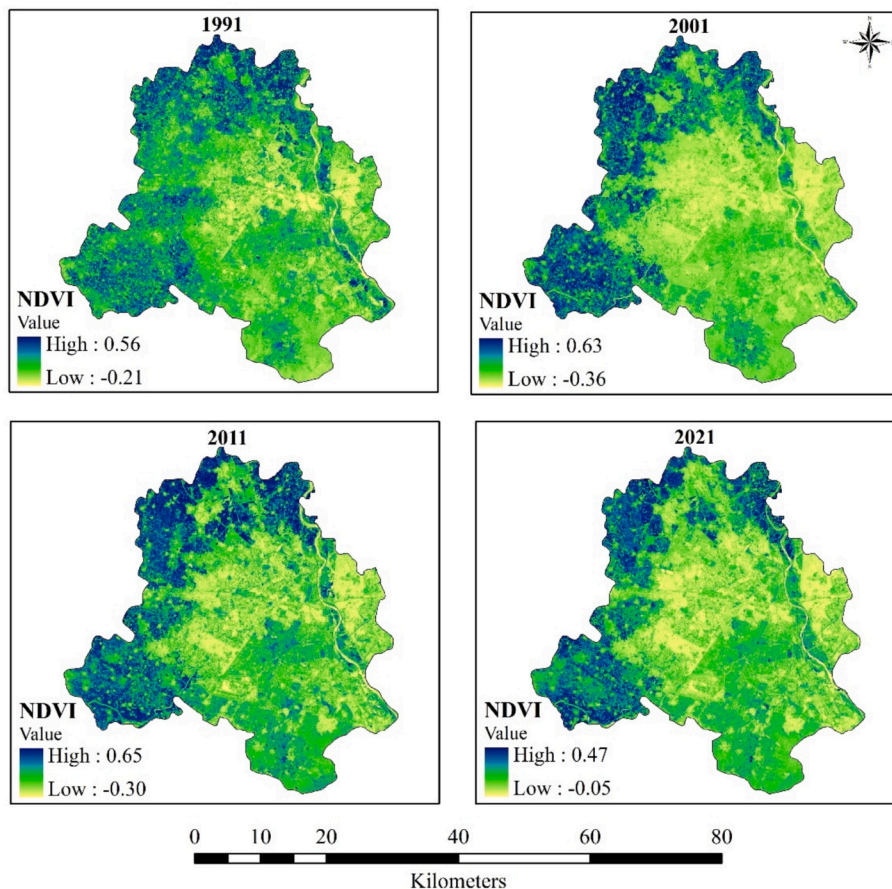


Fig. 3. Spatio-temporal pattern of NDVI across the NCT Delhi for the years 1991, 2001, 2011, and 2021.

3. Results and discussion

3.1. Establishing the vegetation–LST relationship: a foundational analysis

3.1.1. Spatio-temporal pattern of NDVI (1991–2021)

The NDVI was analyzed for the years 1991, 2001, 2011, and 2021 to assess the spatial and temporal dynamics of vegetative cover across the NCT Delhi (Fig. 3). NDVI serves as a robust proxy for vegetative health, biomass density, and green infrastructure intensity, providing baseline ecological context for assessing the thermal impacts of green space dynamics (Dutta et al., 2022).

In 1991, NDVI values ranged from -0.21 to 0.56 , with high vegetation concentration observed in the Ridge areas (North, Central, and South Ridge), Sanjay Van, and along the Yamuna River floodplain. Peripheral rural zones, particularly in Southwest Delhi and near the Asola Bhatti Wildlife Sanctuary, also exhibited dense vegetation, forming natural buffers to urban heat (Shahfahad et al., 2024). By 2001, NDVI values showed a marginal improvement, with the upper limit increasing to 0.63 . This suggests localized greening initiatives, possibly linked to institutional and government afforestation programs. High NDVI values persisted in ecologically sensitive zones like the Delhi Ridge, safeguarded under the oversight of the Delhi Ridge Management Board (1995). However, lower NDVI began to appear along the Outer Ring Road corridors, particularly in West and Northwest Delhi, where rapid urban expansion, infrastructure development, and unauthorized construction were accelerating (Bentinck, 2000). The year 2011 recorded the highest NDVI range (-0.30 to 0.65), indicating a temporary increase in green cover. This anomaly may be attributed to the development of city parks, institutional campuses, and biodiversity parks during the Commonwealth Games phase (2010), when urban greening saw significant investment (Kassens-Noor and Kayal, 2016; Uppal, 2006). Notably, the central institutional belt including Lutyens' Delhi, JNU, IIT Delhi, and Nehru Park, remained robust green zones (Bhalla and Bhattacharya, 2015). However, by 2021, NDVI values declined sharply to a maximum of 0.47 , while the minimum increased to -0.05 , suggesting overall loss of dense vegetation and homogenization of lower NDVI zones. This decline is especially evident in Northwest Delhi, Outer Delhi, and industrial fringe zones like Bawana, Narela, and Najafgarh, which have seen extensive urban and infrastructural development (Mondal et al., 2021). Even parts of East Delhi near the Yamuna embankment show signs of vegetative stress and thinning.

This temporal trajectory underscores a critical urban ecological transition from a vegetated semi-rural cityscape to an increasingly

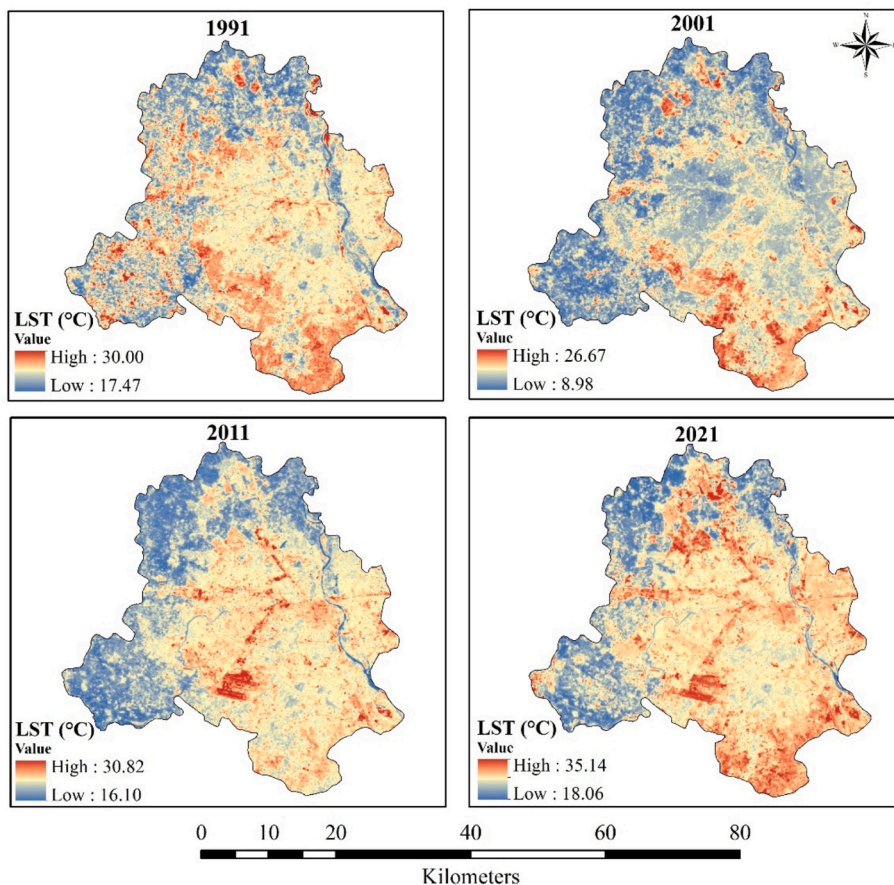


Fig. 4. Spatio-temporal distribution of LST across the NCT Delhi for the years 1991, 2001, 2011, and 2021.

fragmented urban landscape. Despite patches of sustained greenness, the overall decline in high NDVI zones between 2011 and 2021 reflects the pressure of densification and the absence of ecological buffers in many rapidly urbanizing sectors. These spatial transformations are closely tied to changes in surface thermal patterns, as reflected in the corresponding evolution of LST.

3.1.2. Spatio-temporal distribution of land surface temperature (1991–2021)

The spatial distribution of LST across NCT Delhi in 1991, 2001, 2011, and 2021 demonstrates distinct patterns of urban thermal transformation, closely associated with vegetation dynamics and land cover change. These patterns follow the spatio-temporal trends in NDVI, revealing that regions of declining vegetative health and density correspond with areas of elevated LST (Fig. 4). In 1991, LST values ranged from 17.47 °C to 30 °C. Warmer areas were predominantly observed in the southern and central parts of NCT Delhi, including regions around Lajpat Nagar, Okhla Industrial Estate, and parts of Karol Bagh. These zones coincided with dense built-up clusters and lower NDVI values. Cooler patches (below 22 °C) were evident in the Northern Ridge, Sanjay Van, and agricultural peripheries, particularly in Northwest and Southwest Delhi, where vegetation cover was still prominent (Paul and Nagendra, 2015). In 2001, there was a notable dip in the LST range (8.98 °C to 26.67 °C), possibly due to seasonal variation in the data available. However, spatial trends remained consistent: East and Southeast Delhi, especially along the Yamuna belt and Trans-Yamuna areas, began to show signs of thermal intensification (M. Yadav and Kapoor, 2023). Conversely, the northern fringe retained lower LST values, aligned with high NDVI zones from the same year. The LST range expanded again in 2011, peaking at 30.82 °C, with pronounced hotspots emerging in West Delhi, Rohini sub-city, Dwarka, and industrial belts of Bawana and Naraina. This thermal intensification followed increasing concretization and fragmentation of green patches, as seen in satellite and metric-based analyses (Zhou et al., 2022). Despite overall warming, institutions like JNU, Delhi University North Campus, and parts of the Ridge Forest continued to function as localized cool zones an indication of green infrastructure's buffering role. By 2021, LST intensified further, reaching a maximum of 35.14 °C. The spatial spread of high-temperature zones significantly increased, especially in East Delhi, South Delhi, and parts of Najafgarh, which saw a decline in NDVI and a sharp rise in built-up density. Cool zones became more fragmented and localized, notably around biodiversity parks, large institutional campuses, and residual agricultural lands near NCT Delhi's border (Shahfahad et al., 2024). The minimum temperature, though slightly higher than in 2011, indicates a general warming trend across the city, with even vegetated zones experiencing thermal stress.

This spatial and temporal evolution of LST demonstrates its inverse association with the dynamics of vegetative cover and green space configuration. The observed spatial patterns suggest that LST variations are not uniformly distributed but are strongly influenced by the structure and persistence of green spaces. To quantify the strength and consistency of this relationship, a regression analysis was conducted between NDVI and LST over the same time period.

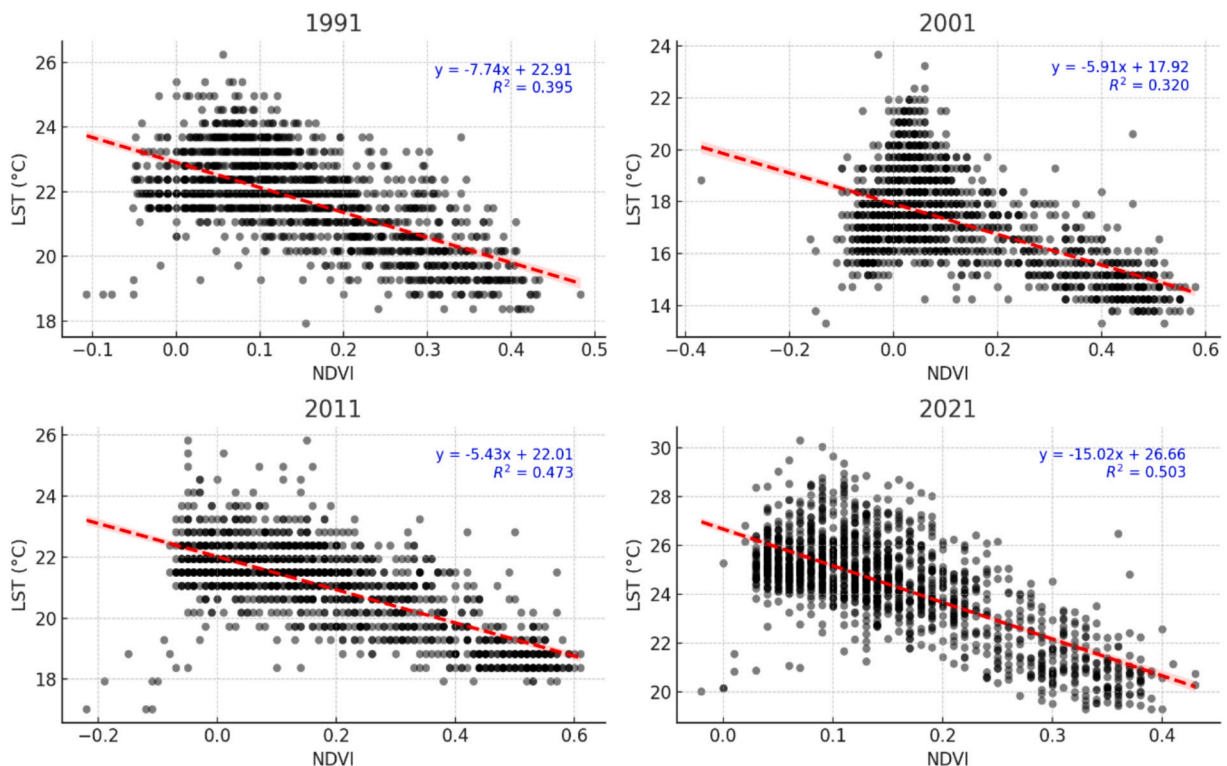


Fig. 5. Comparative regression analysis between NDVI and LST for the years 1991, 2001, 2011, and 2021 in the NCT Delhi.

3.1.3. NDVI–LST regression analysis

To quantitatively assess the influence of vegetative cover on LST, a regression analysis was conducted between the NDVI and LST for the years 1991, 2001, 2011, and 2021. To reinforce the visually observed inverse relationship between vegetation cover and LST, this approach provided a quantitative basis with statistical validation. The analysis revealed a persistent and strengthening negative correlation between NDVI and LST over the study period (Fig. 5). In 1991, the regression equation was $LST = -7.74 \times NDVI + 22.91$, with a coefficient of determination (R^2) of 0.39, indicating a moderate inverse relationship. This suggested that even during early stages of urban development, vegetated areas contributed meaningfully to surface cooling (Hamada et al., 2013). In 2001, the strength of this relationship weakened slightly, with the slope decreasing to -5.91 and R^2 falling to 0.32. This reduction may be attributed to localized urban fragmentation and a transitional phase in land use patterns, especially in the city's eastern and peripheral zones. By 2011, the relationship regained strength ($R^2 = 0.47$), with the regression slope of -5.43 again indicating a stable inverse trend. This improvement coincided with short-term urban greening initiatives and an increase in institutional and recreational green spaces implemented during the Commonwealth Games infrastructure phase. These green patches, although fragmented, continued to exert localized cooling effects. The 2021 regression demonstrated the most significant outcome, with a steep slope of -15.02 and an R^2 value of 0.50 the highest across all observed years. This sharp gradient underscores the intensified thermal impact of vegetative loss. In highly urbanized and densely built environments, even marginal increases in NDVI were associated with substantial reductions in LST, highlighting the amplified role of vegetation as a thermal buffer in later stages of urban growth.

These results highlight a temporally strengthening inverse correlation between NDVI and LST, with the relationship becoming more pronounced as urban heat intensifies. The increasing slope magnitude and R^2 values suggest that vegetation's cooling function becomes more prominent under conditions of accelerated urban expansion and ecological degradation (C. Wang et al., 2023). To further characterize this thermal behaviour across the urban fabric, a class-wise analysis of LULC-based LST deviation was performed, enabling a differentiated view of how specific land use types contribute to or buffer against urban heat accumulation.

3.1.4. LULC-wise ΔLST analysis (1991–2021)

Following the NDVI–LST regression analysis, a land use based thermal deviation assessment was conducted to further verify the inverse relationship between green space and LST (Kayet et al., 2016). ΔLST , defined as the difference between the average temperature of each LULC class and the overall mean LST, serves as a robust indicator of the relative thermal behaviour of different land cover types as shown in (Fig. 6).

Across all years, built-up and barren land consistently exhibited positive ΔLST values, confirming their contribution to urban heating (Morabito et al., 2016; Roy et al., 2011). Built-up areas showed a steady increase from $+1.3^\circ\text{C}$ in 1991 to $+2.1^\circ\text{C}$ in 2021, following rapid urban expansion and surface sealing. In contrast, vegetation and forest classes exhibited persistently negative ΔLST values, with forest cooling increasing from -1.1°C to -1.6°C , and general vegetation from -0.6°C to -1.2°C in the same period. Water bodies demonstrated the strongest cooling capacity ($\Delta LST < -1.8^\circ\text{C}$), consistent with recent evidence that the spatial geometry and continuity of aquatic systems play a critical role in enhancing local thermal regulation (Ampatzidis et al., 2023).

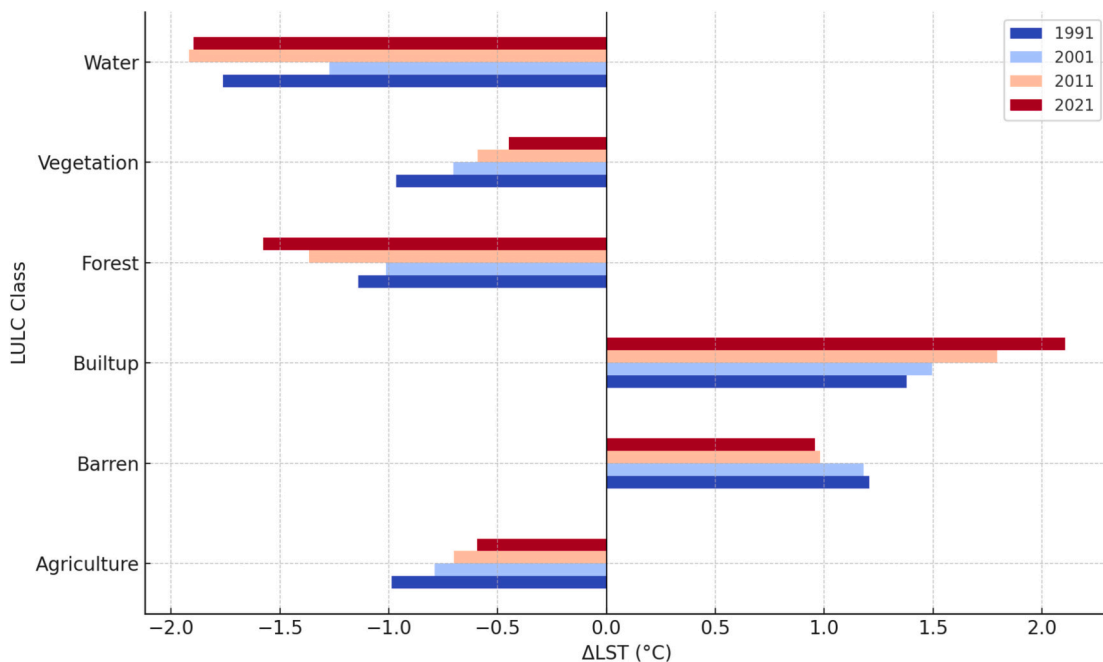


Fig. 6. Temporal variation in mean LST (ΔLST) across major Land Use and Land Cover (LULC) classes in NCT Delhi for the years 1991, 2001, 2011, and 2021.

These findings quantitatively confirm that vegetated land uses including both forest and general vegetation exert a consistent cooling influence on LST, while built-up and barren areas contribute positively to urban heat accumulation. To further examine the spatial characteristics that govern this thermal behaviour, the study applies a suite of landscape metrics to the vegetation class. This analysis captures the composition, shape complexity, spatial configuration, and connectivity of green patches, enabling identification of the most influential spatial attributes associated with LST regulation.

3.2. Vegetation patch structure and its thermal implications

To investigate the role of green space structure in regulating LST, a suite of landscape metrics was applied to the vegetation class in NCT Delhi for the year 2021 as shown in (Fig. 7).

These metrics derived using Fragstats capture key spatial dimensions such as area dominance (PLAND, LPI), shape complexity (FRAC, MSI), spatial cohesion (AI, CONTAG), fragmentation (NP, ED), and inter-patch proximity (ENN-MN). Their spatial distribution reveals critical insights into the ecological configuration of urban vegetation and its influence on thermal conditions (Y. Zhang et al., 2022). The PLAND and LPI maps reveal a pronounced concentration of large, contiguous green patches in the southern and central parts of NCT Delhi, particularly around the Ridge areas, JNU, Sanjay Van, and other institutional zones. These zones coincide with previously identified LST cool pockets, underscoring the moderating effect of green patch dominance. In contrast, peripheral zones in

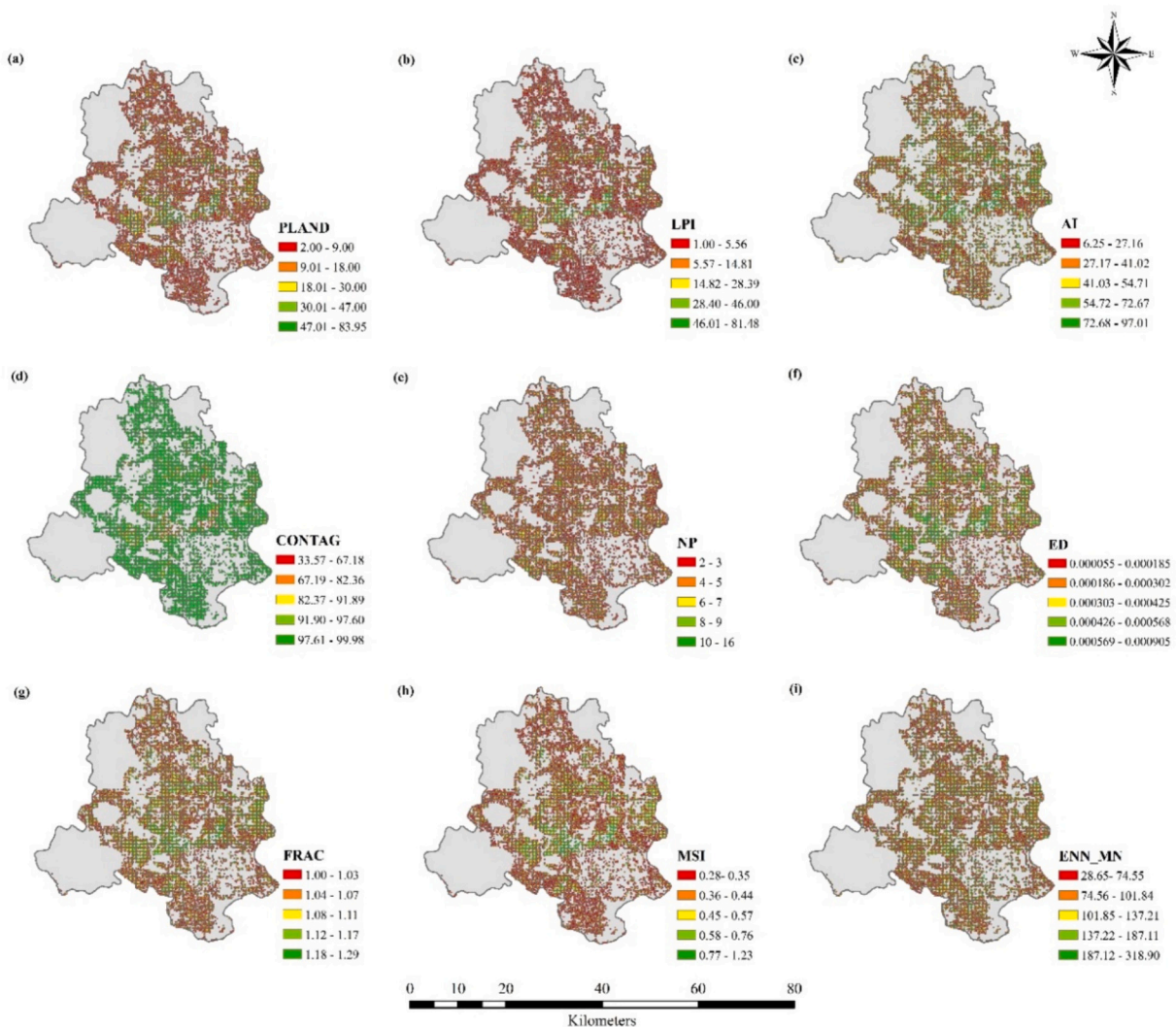


Fig. 7. Spatial distribution of urban green space landscape metrics across NCT Delhi in 2021: (a) Percentage of Landscape (PLAND), (b) Largest Patch Index (LPI), (c) Aggregation Index (AI), (d) Contagion Index (CONTAG), (e) Number of Patches (NP), (f) Edge Density (ED), (g) Fractal Dimension Index (FRAC), (h) Mean Shape Index (MSI), and (i) Euclidean Nearest Neighbour-Mean Distance (ENN_MN). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

West and North Delhi exhibit low PLAND and fragmented LPI values, aligning with high-LST zones observed in preceding sections. AI and Contagion (CONTAG) values were highest in southern institutional and forested regions, indicating well-clustered vegetation. Conversely, low AI and CONTAG scores in industrial and residential expansion zones such as Narela, Bawana, and Najafgarh suggest spatial disaggregation and ecological isolation of patches structural attributes known to reduce cooling potential.

The NP and ED maps indicate high fragmentation in outer Delhi, especially in urban fringe zones under development pressure. These areas, characterized by numerous small and disconnected vegetation patches, reflect low thermal resilience due to increased edge effects and reduced core vegetative function. This aligns with LST hotspots in 2021, reinforcing the role of fragmentation in exacerbating urban heat stress (Maimaitiyiming et al., 2014). Shape-related metrics FRAC and MSI further highlight morphological complexity in central Delhi's institutional greens and urban parks, indicating more stable and ecologically functional vegetation structures. In contrast, low FRAC and MSI values in peripheral wards indicate oversimplified, irregular patches with reduced ecological performance. Finally, ENN-MN metric confirms high inter-patch distances in barren and low-income settlement zones, particularly in East and Northwest Delhi. These disconnected vegetative remnants contribute little to localized cooling due to their spatial isolation and limited capacity for ecological flow.

Collectively, the spatial analysis underscores that compact, aggregated, and morphologically complex vegetation patches concentrated in the Ridge and institutional greens are structurally optimized to mitigate LST. In contrast, fragmented, irregular, and

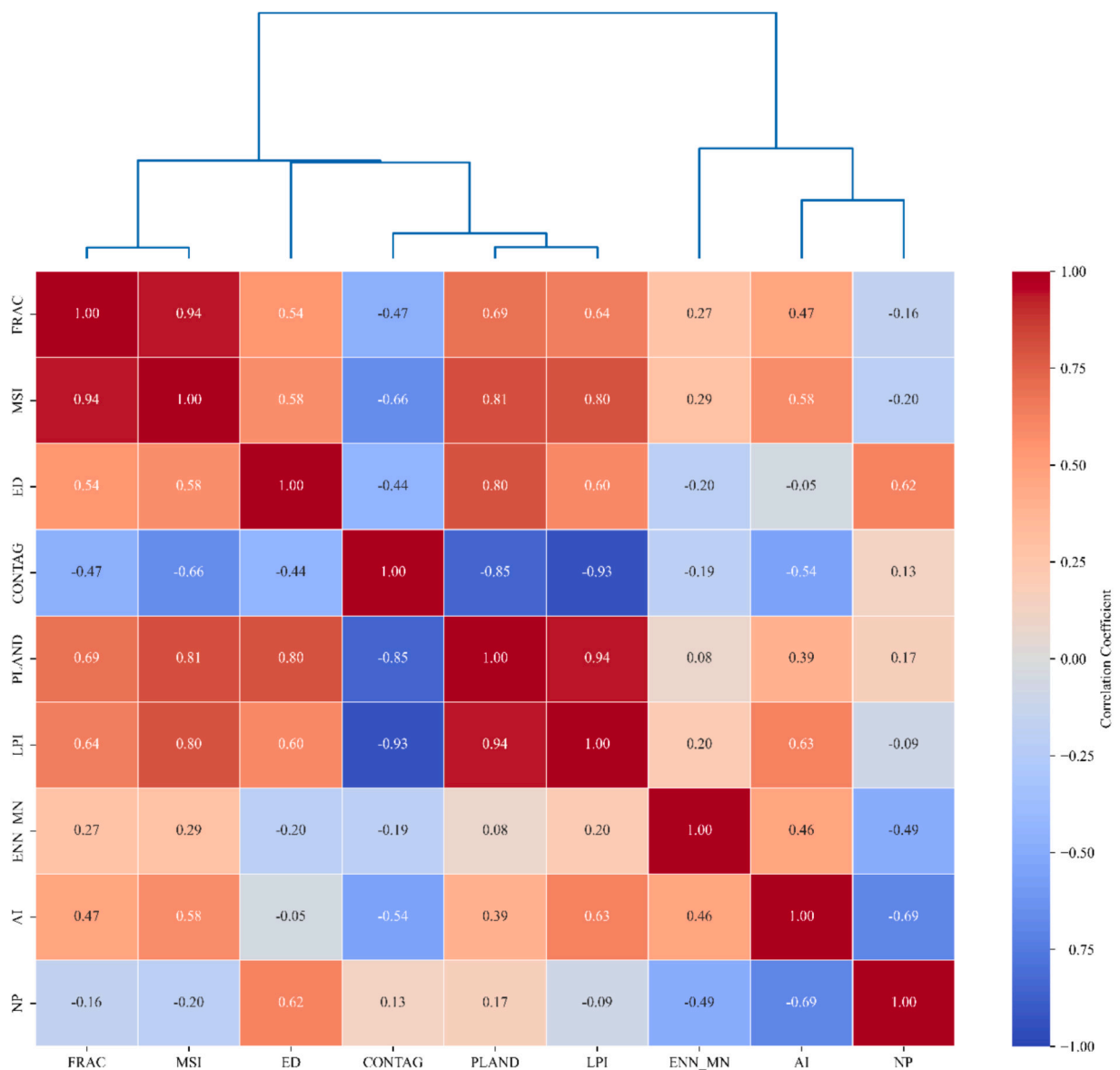


Fig. 8. Correlation plot of green space metrics. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

spatially isolated patches dominate peri-urban and industrial zones, aligning closely with observed thermal hotspots. These findings reinforce and spatially extend the NDVI–LST relationship, highlighting that it is not just the presence but the structural integrity and spatial cohesion of green space that govern its effectiveness in urban heat mitigation (Li et al., 2012; W. Liu et al., 2022). This has direct implications for spatially targeted green infrastructure planning and ecological zoning under climate-sensitive urban development frameworks.

3.3. Machine learning model evaluation and diagnostic analysis

3.3.1. Correlation & multi- collinearity diagnostic

To evaluate interdependencies among the nine vegetation-based landscape metrics, a Pearson correlation matrix and VIF analysis were conducted (Oke et al., 2022). This diagnostic step ensured that multicollinearity would not compromise the interpretability or stability of subsequent ML-XAI approach (Chan et al., 2022). The correlation matrix (Fig. 8) revealed several strong positive correlations, most notably between FRAC and MSI ($r = 0.94$), and between PLAND and LPI ($r = 0.94$). These strong correlations are ecologically justified, as FRAC and MSI both represent aspects of patch shape complexity, and in highly urbanized environments like NCT Delhi, patches with more irregular or elongated forms tend to co-occur in mixed-use and fragmented areas (Mabrouk et al., 2024). Similarly, PLAND and LPI are naturally related areas with high overall vegetation coverage (PLAND) are often dominated by one or more large patches (LPI), especially in contiguous forested or institutional green zones such as the Ridge or JNU. Another notable correlation was observed between PLAND and MSI ($r = 0.81$), which reflects the fact that larger green areas tend to exhibit more complex geometries in urban matrices (Grafius et al., 2018). However, such relationships do not imply collinearity in terms of predictive contribution, as these metrics capture different spatial facets.

Conversely, strong negative correlations were observed between CONTAG and both PLAND ($r = -0.85$) and LPI ($r = -0.93$). This inverse relationship reflects how, in rapidly urbanizing or peri-urban zones, high green patch dominance often comes at the cost of overall landscape cohesion. For instance, a large but isolated green patch like Sanjay Van may elevate PLAND or LPI but reduce CONTAG due to surrounding fragmentation (Nagendra et al., 2012). This reflects NCT Delhi's ecological heterogeneity where structural dominance does not necessarily imply connectivity or cohesion.

The VIF analysis further supported the inclusion of all nine metrics in the modelling process (Table 4). Although ED (9.07) and PLAND (9.05) were close to the upper multicollinearity threshold, they remained within acceptable bounds. These values are consistent with the landscape composition of NCT Delhi, where dense vegetation patches (PLAND) often come with complex edge structures (ED) due to urban interfaces. All other metrics exhibit VIF values of less than 2 (1.04 to 1.08), indicating low inter-predictor redundancy and independence in their spatial behaviour. Therefore, their inclusion is not only statistically valid but ecologically necessary to capture the multidimensional nature of green space–LST interactions.

3.3.2. Model performance evaluation

To predict LST based on vegetation patch structure metrics, three ML models GBM, DRF, and DL were evaluated using the H2O AutoML platform with appropriate training and validation splits. The comparative results are illustrated in (Fig. 9) as radar plots displaying three evaluation metrics: R^2 , RMSE and MAE. Among the three, the GBM model consistently outperformed the others, achieving the highest explanatory power ($R^2 = 0.8859$), along with the lowest RMSE (0.0340) and MAE (0.0222), indicating superior predictive accuracy and residual minimization. The DL and DRF models yielded comparable yet lower performances; DL attained an R^2 of 0.8818 and RMSE of 0.0346, while DRF recorded $R^2 = 0.8806$ and RMSE = 0.0348. The out-of-sample results on the hold-out test set were similar, showing strong agreement in predictions of the developed models. Actual versus predicted plots, residual versus observed values, and residual density distributions were analyzed to check calibration and variance. Relative-error density, measured using Average Absolute Percentage Relative Error (AAPRE), captured proportional error patterns in the subsequent sections. The diagnostics showed minimal bias and consistent variance, confirming reliable and stable model performance. Although GBM, DRF, and DL achieved comparable predictive accuracy ($R^2 \approx 0.88$), the GBM was selected as the final model for subsequent application of XAI techniques. Its balance between predictive precision, computational efficiency, and explainability (via SHAP and ICE analyses) ensures robust yet interpretable insights. The minimal gain expected from more complex ensemble or hybrid architectures does not justify the added complexity or reduced transparency, supporting the preference for a simplified yet accurate GBM model. Despite the modest differences, GBM demonstrates greater robustness and generalization capability (Friedman, 2001; Natekin and Knoll, 2013), making it

Table 4
Multicollinearity assessment of landscape metrics using Variance Inflation Factor (VIF).

S. No.	Landscape Metric	Abbreviation	VIF Value	Interpretation
1	Percentage of Landscape	PLAND	9.05	Acceptable, close to threshold
2	Edge Density	ED	9.07	Acceptable, close to threshold
3	Largest Patch Index	LPI	1.05	No multicollinearity
4	Euclidean Nearest Neighbour Mean	ENN_MN	1.06	No multicollinearity
5	Number of Patches	NP	1.04	No multicollinearity
6	Contagion Index	CONTAG	1.04	No multicollinearity
7	Fractal Dimension Index	FRAC	1.08	No multicollinearity
8	Mean Shape Index	MSI	1.06	No multicollinearity
9	Aggregation Index	AI	1.08	No multicollinearity

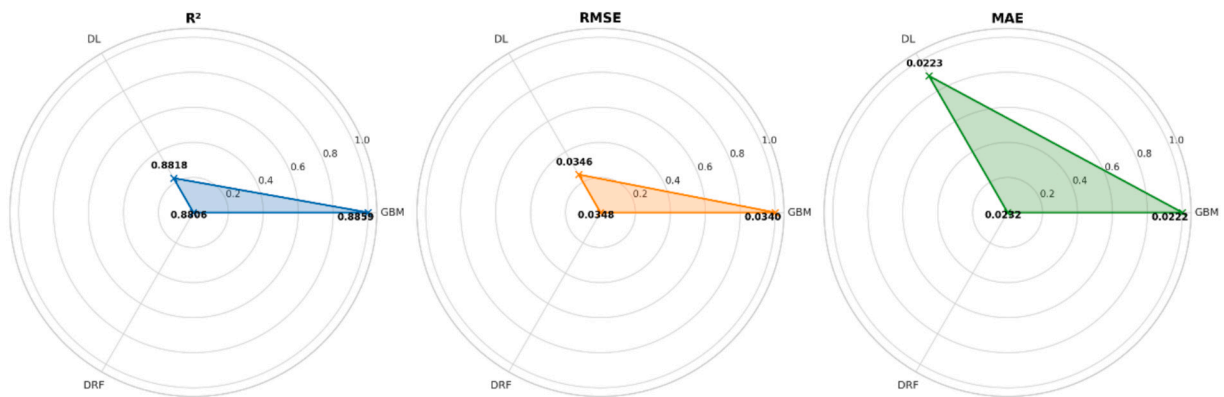


Fig. 9. Radar plots comparing the performance of three machine learning models Gradient Boosting Machine (GBM), Deep Learning (DL), and Distributed Random Forest (DRF) based on their R^2 , RMSE, and MAE.

the most suitable model for subsequent residual diagnostics and interpretability analysis. Moreover, GBM's compatibility with XAI techniques enhances transparency by enabling detailed visualization of variable influence and interactions (Lundberg and Lee, 2017; Goldstein et al., 2015), thereby linking predictive accuracy with explainable modelling.

The results also illustrate a classic bias–variance trade-off indicating that increasing capacity can fit complex structure but risks overfitting when data are limited. Here, regularized ensembles achieved accuracy on par with deeper architectures, and concordant XAI patterns across models support robust ecological inference. For policy translation, it is therefore emphasized that the simplest accurate models like GBM shall be preferred over complex DL architectures.

3.3.3. Residual diagnostic and predictive reliability of ML models

To complement traditional accuracy metrics and ensure the robustness of the selected models, a comprehensive residual diagnostics analysis was performed on the top three algorithms i.e., GBM, DRF, and DL as shown in (Fig. 10).

The GBM model demonstrates the most desirable residual characteristics. Its residuals are narrowly centered around zero with a sharp, symmetric distribution, indicating low prediction bias and homoscedastic variance. The residual scatterplot reveals no apparent funneling or curvature, suggesting that errors are consistent across the range of predicted LST values. The density plot further confirms

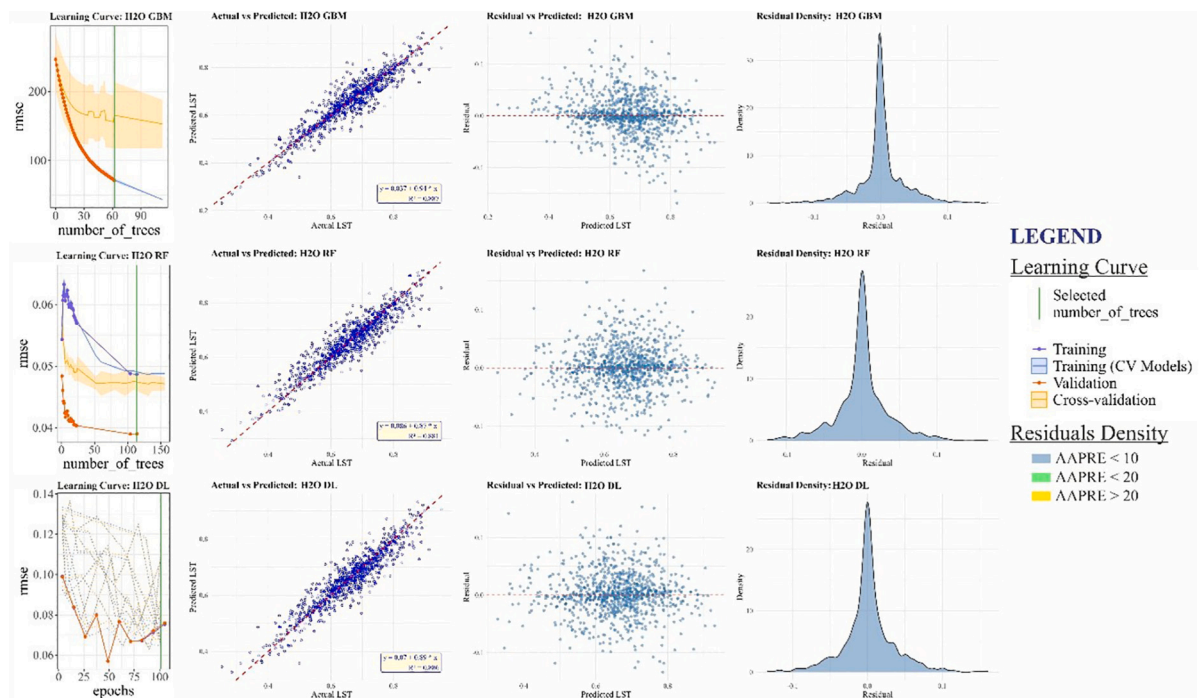


Fig. 10. Comparative diagnostics of machine learning models: learning curves, actual vs. predicted plots, residual scatterplots, and residual density estimates.

the stability of GBM, showing a tall, peaked distribution indicative of minimal dispersion and a high degree of model confidence. In contrast, the DRF model, although still robust, exhibits a slightly broader residual spread. While the residuals are generally centered near zero, the presence of minor asymmetry and heavier tails in the density plot implies a comparatively higher prediction uncertainty. The DRF model's predicted values are mostly close to the actual values, but the points are more spread out than those of the GBM model, especially at higher LST levels. The DL model performs moderately well but shows greater variability in both its learning curve and residual pattern. The residuals for DL appear more dispersed across predicted values, suggesting sensitivity to non-linear fluctuations. The residual density is flatter relative to GBM and DRF, denoting broader prediction errors. Moreover, the learning curve for DL lacks the smooth convergence observed in the ensemble models, potentially due to the limited dataset size and overfitting tendencies of deep networks when applied to structured tabular data.

The residual diagnostics reinforce the selection of GBM as the most stable and generalizable model for LST prediction in the context of urban vegetation metrics. Its tighter residual bounds and consistent learning behaviour underscore its suitability for subsequent application of XAI techniques.

3.4. Identifying key vegetation landscape metrics driving cooling effect on LST using explainable artificial intelligence (XAI) techniques

The SHAP (beeswarm) plot (Fig. 11) provides a global interpretation of the influence of vegetation landscape metrics on LST predictions across the study area. Among all metrics, ED exhibits the strongest positive influence, indicating that higher vegetation fragmentation contributes to increased LST. This is ecologically intuitive, as greater ED exposes more vegetated boundaries to solar radiation and surrounding built-up heat, increasing sensible heat flux and weakening latent heat exchange. Fragmented green spaces also disrupt the continuity of evapotranspiration and air circulation, thereby diminishing their capacity to dissipate the stored heat. In simple terms, disconnected or highly segmented green spaces lose their collective cooling capacity, leading to hotter local conditions. This pattern is particularly evident in the densely built-up zones of East and North-West Delhi, where small, scattered patches of green space are unable to offset the accumulated heat (Pramanik and Punia, 2020). Similar configuration–temperature relationships have been documented globally Myint et al. (2015) demonstrated that dispersed vegetation structures in Phoenix (United States of America) intensified surface heating; Liu et al. (2024) found that landscape fragmentation in Nanchang (China) increased LST; and Jia et al.

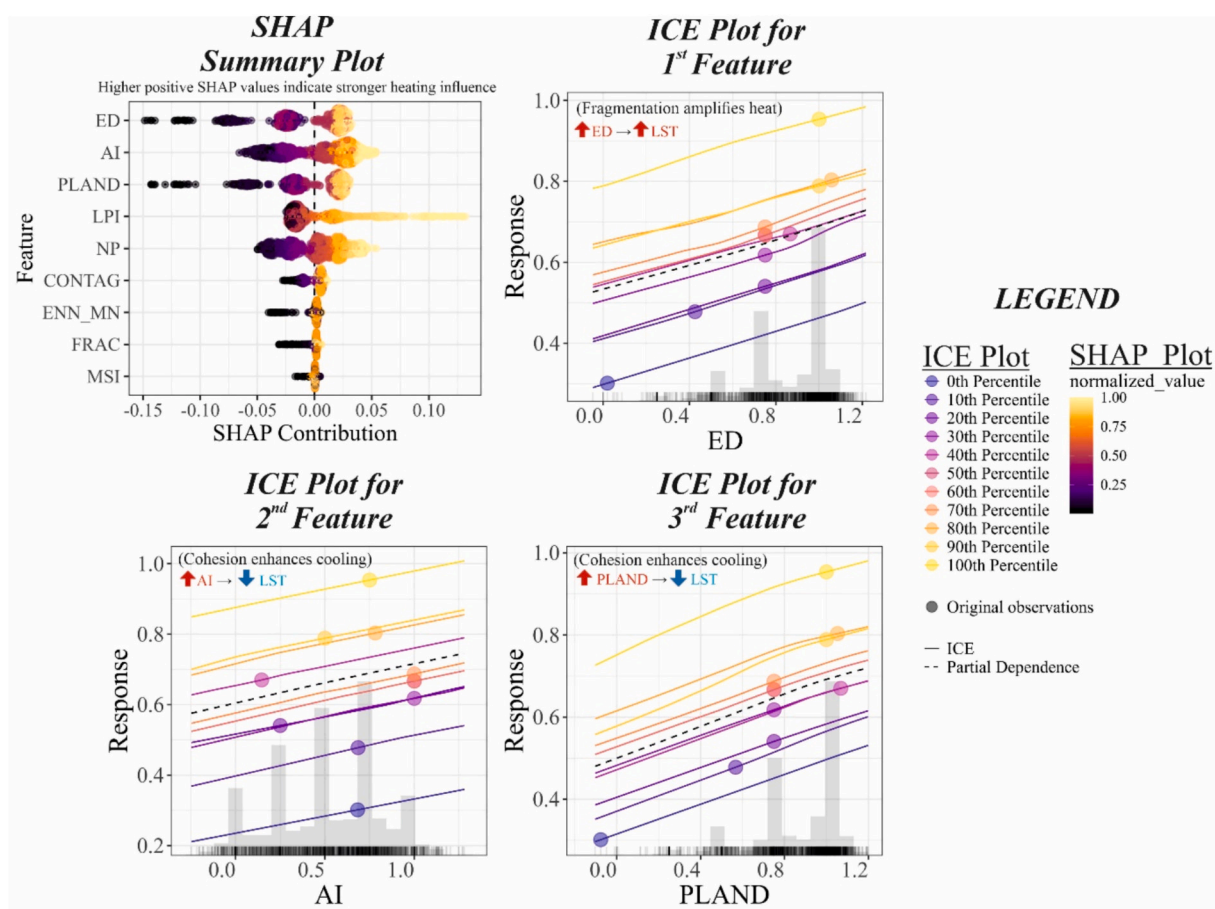


Fig. 11. SHAP summary and ICE plots showing the influence of vegetation landscape metrics on predicted LST in NCT Delhi.

(2022) reported that more connected and aggregated vegetation patches consistently moderated heat intensity in Jiaozuo (China). In contrast, both Percentage of Landscape (PLAND) and Aggregation Index (AI) exhibit negative SHAP contributions for higher values, signifying that greater vegetated area and spatially cohesive green patterns are linked to cooler surface conditions (A. Chen et al., 2014b). Ecologically, this reflects the efficiency of continuous vegetation in facilitating evapotranspiration, maintaining soil moisture, and reducing radiant heat absorption through canopy shading and surface albedo moderation. Comparable findings from Harare (Zimbabwe) (Kowe et al., 2021) further confirm that the spatial configuration and connectivity of green spaces substantially regulate local thermal environments. These relationships align with field observed cooling patterns in major green zones such as Lodhi Garden, Nehru Park, and the Delhi Ridge, where dominant and connected vegetation markedly moderates urban heat (Weng et al., 2004). Other metrics like LPI and NP offer moderate contributions, while CONTAG, ENN_MN, FRAC, and MSI show limited influence, reinforcing the idea that spatial coherence and total vegetation share are more decisive than fragmentation count or shape complexity in regulating urban temperatures.

To explore the localized and percentile-specific impact of the top predictors, ICE plots were used for ED, AI, and PLAND. The ICE plot for ED reveals a consistent and strong upward trend across all percentiles, indicating that as ED increases, predicted LST rises steadily. In simpler terms, more fragmented vegetation with excessive edges intensifies surface heating, as small, disconnected green patches fail to retain or disperse cool air effectively. This pattern is evident in urban enclaves such as Jahangirpuri, Uttam Nagar, and parts of West Delhi, where fragmented green spaces provide minimal cooling influence. In contrast, the ICE curve for AI shows a distinct non-linear relationship with LST. While lower aggregation levels do little to influence temperature, once AI crosses a moderate threshold, its impact on reducing LST becomes more substantial. This threshold behaviour emphasizes the importance of vegetative continuity, as found in the ridge forests, institutional campuses like JNU, and planned sectors of South Delhi, where aggregated vegetation blocks offer larger buffer zones against urban heat. The ICE plot for PLAND displays a smooth, inverse relationship with LST, where increasing vegetation coverage results in uniform and significant temperature decline across all percentiles. In simple terms, the greener cover a locality has, the cooler it becomes, regardless of how vegetation is spatially arranged. This is particularly evident in regions like Hauz Khas, Siri Fort, and Lutyens' Delhi, where higher landscape coverage correlates with notably lower LST values. The consistent downward trend across percentile bands suggests that increasing the total area of vegetation regardless of configuration remains an effective intervention for thermal mitigation.

Together, the SHAP and ICE-based explainability analysis confirms that urban cooling in NCT Delhi is most effectively driven by increasing vegetation cover (PLAND), reducing fragmentation (ED), and promoting spatial aggregation (AI). These three metrics emerge as the dominant spatial determinants of LST variation, highlighting that both vegetation quantity and spatial integrity are critical for mitigating urban heat. The findings underscore the need for spatially strategic urban greening policies, where not just the quantity but the configuration of vegetation are optimized to mitigate rising heat stress. Consequently, urban planning interventions should prioritize cohesive green corridors, restoration of contiguous green belts, and restriction of highly fragmented vegetative zones in densely populated urban cores. As climate adaptation becomes central to urban policy, these insights provide a scientifically grounded framework for designing green infrastructure that is both ecologically functional and thermally resilient.

4. Conclusion

This study presents a comprehensive spatial framework to assess how the structure of vegetation landscapes helps reduce urban heat in NCT Delhi. By combining Fragstats-derived metrics with ML-based regression and XAI techniques, it identifies key spatial factors influencing LST and offers a replicable approach to urban thermal resilience. The findings of this study lead to the following major conclusions, offering valuable insights regarding the importance of urban green spaces in NCT Delhi:

- **Influence of Vegetation Landscape Metrics on LST:** Vegetation landscape structure has a significant influence on LST in the region of NCT Delhi. The fragmented green spaces represented by the ED increase the surface heating by increasing edge exposure and disrupting evapotranspiration processes. Cohesive vegetation cover represented by PLAND and AI effectively reduce the urban heat through enhanced canopy shading, evapotranspiration, and ecological connectivity. XAI results corroborate that ED is positively related with LST while PLAND and AI exhibit a negative relationship, underscoring the critical role of vegetation configuration in mitigating urban heat.
- **Spatial Variations Across NCT Delhi:** Heat-prone areas like East Delhi (Shahdara, Seelampur) and Northwest Delhi (Narela, Bawana, Rohini Extension) exhibited high ED and low PLAND values, making them priority zones for intervention. Urban greening in these sectors should focus on developing cohesive green belts and connected vegetation corridors along the Yamuna floodplain, industrial peripheries, and major transport corridors such as NH-44 and Outer Ring Road. Conversely, thermally stable zones such as Lutyens' Delhi, South-Central Delhi (Chanakyapuri, Lodhi Estate), and institutional-green complexes near the Ridge and Sanjay Van demonstrated high PLAND and AI, validating the effectiveness of large, continuous, and aggregated green spaces in mitigating urban heat.
- **Superior performance of GBM:** GBM emerges as the best performing and robust ML model for predicting the LST with a high predictive accuracy and low residuals. This confirms the model's robustness and generalizability for capturing spatio-temporal LST variations in a complex urban environment.
- **Policy and Planning Implications:** The study highlights that landscape configuration metrics particularly ED, PLAND, and AI should be prioritized in ward-level greening policies, zoning regulations, and climate adaptation plans. Instead of isolated green patches, planning efforts should emphasize establishing connected green corridors and vegetated linkages between existing parks and institutional greens such as the Lodhi Garden – Nehru Park – Delhi Ridge continuum in Central–South Delhi, and between

Sanjay Van, Hauz Khas, and adjacent forest reserves. In the highly heat-stressed zones of East Delhi (e.g., Shahdara, Seelampur) and North-West Delhi (e.g., Narela, Bawana industrial clusters), ward-level interventions should prioritize micro-greening measures such as roadside tree avenues, green medians, and vertical or rooftop greening to offset thermal accumulation and enhance local cooling. These measures can be operationalized through integration with existing urban frameworks, including the Delhi Master Plan 2041, the National Urban Greening Mission, and the Smart Cities Programme, ensuring that connectivity-based greening becomes a mandated planning criterion rather than a voluntary initiative. Collectively, these policy measures translate the model's spatial insights into actionable insights for climate-sensitive urban design and ecosystem-based adaptation in Delhi.

Overall, this research contributes a first-of-its-kind, XAI integrated framework for understanding the spatial drivers of urban heat in NCT Delhi. It reinforces the need for spatially informed greening strategies that move beyond generic area-based targets to emphasize structural coherence, connectivity, and ecological continuity. These insights offer a scientifically grounded foundation for enhancing urban resilience against heat stress and can be scaled to other Indian megacities facing similar challenges of rapid urbanization and climatic extremes. Despite offering important insights into the role of urban green space structure in regulating LST across NCT Delhi, this study has certain limitations. Firstly, the analysis was limited to green space metrics derived solely from the vegetation class, excluding the potential contribution of tree canopy density, vertical green infrastructure, or small-scale urban gardens due to data constraints. Secondly, the temporal scope focused on four discrete years without accounting for seasonal variations in vegetation cover and LST, which could further enrich understanding. Thirdly, this study uses k-fold cross-validation, early stopping, and an external hold-out set but did not include spatial cross-validation, which can reduce leakage from spatial autocorrelation. Future work can integrate block or spatial CV, bootstrap or conformal uncertainty intervals, and MC-dropout for DL to quantify pixel- or segment-level predictive uncertainty. Future research can also build upon this work by incorporating high-resolution spatial and temporal data, integrating LiDAR-derived canopy height models, or utilizing multi-seasonal satellite imagery to account for intra-annual variations. The inclusion of socioeconomic and built-environment variables alongside ecological metrics could also offer a more comprehensive urban climate assessment. Furthermore, coupling XAI with geospatial simulations, such as CA-Markov or cellular automata, could aid in forecasting urban LST dynamics under different urban planning scenarios. Such advanced studies would significantly enhance research and serve as decision-support tools for climate-resilient urban design and policy interventions.

CRedit authorship contribution statement

Manish Kumar: Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Sourav Bhadwal:** Writing – review & editing, Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Netrananda Sahu:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Formal analysis, Conceptualization.

Declaration of competing interest

The authors unanimously declare that there is no Conflict of Interest.

Data availability

Data will be made available on request.

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