# Dealing with Spatial Heterogeneity: A Graph Neural Network-based Domain Adaptation Framework in Urban Heat Prediction

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GISRUK 2026

**Summary**

Land Surface Temperature (LST) is critical in understanding urban heat dynamics and their implications for sustainability, health, and planning. However, accurately predicting LST across diverse urban areas remains challenging due to spatial heterogeneity arising from variations in urban morphology, land cover, and local climate. This study introduces a Graph Neural Network-based Domain Adaptation (GNN-DA) framework that leverages graph-based spatial representations and adversarial learning to align feature distributions across cities. Trained on data from Singapore, the model demonstrates strong predictive performance in Malacca, achieving high $R^2$ scores and low Root Mean Square Error (RMSE), and shows reasonable generalisability to Melbourne and Bristol during summertime, underscoring the framework's capacity to transfer knowledge across diverse urban contexts.

**KEYWORDS:** Spatial Heterogeneity, GeoAI, Urban Heat, Adversarial Training.

## 1 Introduction

Urban heat, reflected in land surface temperature (LST), is a critical environmental issue exacerbated by urbanisation and climate change (Corburn, 2009). Accurate LST prediction is essential for

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sustainable urban planning, public health, and environmental management (Rizwan et al., 2008). Despite efforts to develop universal models for cross-city urban heat prediction (Bechtel et al., 2015; Varentsov et al., 2023), spatial heterogeneity, arising from variations in urban morphology, land cover, socio-economic factors, and climatic conditions, presents significant challenges (Gao et al., 2022; Liao et al., 2021). Traditional machine learning models trained on single-region data struggle to generalise, leading to oversimplified predictions and reduced applicability in diverse urban contexts (Li et al., 2024a,b; Mai et al., 2024). Therefore, robust frameworks are required to capture spatial dependencies and adapt to city variations.

Graph Neural Networks (GNNs) provide a promising approach, as they encode local and global spatial dependencies through graph-based representations of urban data (Liu and Biljecki, 2022; Mai et al., 2022; Liu et al., 2024). By modelling interconnected structures such as road networks, building footprints, and green spaces, GNNs are particularly suited to spatially heterogeneous data. However, domain shifts, including differences in feature distributions, graph structures, and environmental conditions, pose significant challenges when applying GNNs across cities (HassanPour Zonoozi and Seydi, 2023). To address such a challenge, domain adaptation (DA) techniques have emerged as a powerful method to align feature distributions and enable effective adaptation to new geographic contexts.

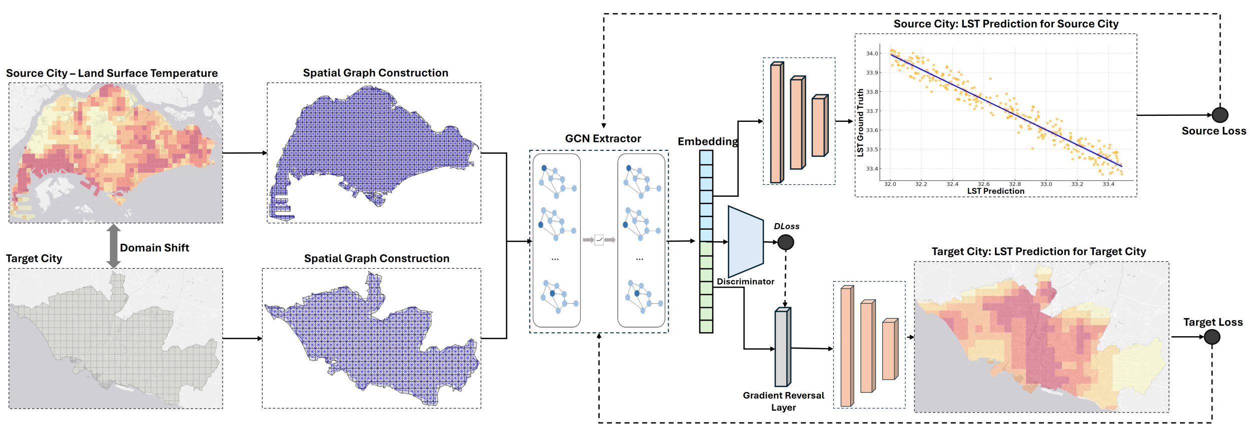


Figure 1: The overall framework.

This study proposes a Graph Neural Network-based Domain Adaptation (GNN-DA) framework to deal with spatial heterogeneity in urban heat prediction. The framework employs GNNs to model urban spatial relationships and integrates domain adaptation techniques to bridge gaps between source and target domains. A customised Gradient Reversal Layer (GRL) facilitates adversarial training by aligning feature distributions across cities using spatial similarities, enabling the model to generalise effectively across urban environments with diverse spatial characteristics.

The GNN-DA framework was trained using LST data from Singapore and tested on cities with varying spatial and climatic characteristics: Malacca (Malaysia), Melbourne (Australia), and Bristol (UK). Results showed strong performance in cities with moderate domain shifts, such as Malacca, and reasonable generalisability in cities with significant domain shifts, such as Melbourne and

Bristol, for summertime LST predictions.

## 2 Method and Case Studies

The overall framework of the proposed GNN-DA is illustrated in Figure 1, which addresses the domain adaptation challenge for predicting LST between cities with domain shifts. In this section, we will detail each component of the framework and also the study areas that we tested.

### 2.1 Spatial Graph Construction

Spatial graph construction is central to the GNN-DA framework, and the graphs are constructed for the source and target cities to capture their respective spatial structures and relationships. Urban areas are represented as uniform $1000 \times 1000$-meter grid cells, each corresponding to a graph node. Attributes for nodes include urban morphology, environmental indicators, and population density (see Section 2.3). Edges, based on Queen's spatial weights, connect adjacent nodes, capturing local spatial dependencies. While regular grid cells are used here for simplicity, the framework is flexible and can be extended to handle irregular spatial units such as parcels or administrative boundaries.

### 2.2 Graph Neural Network-based Domain Adaptation

The GNN-DA framework models spatial dependencies using graph representations and aligns feature distributions across cities via adversarial domain adaptation. Let $G_s = (V_s, E_s)$ and $G_t = (V_t, E_t)$ represent the source and target city graphs, where $V_s, V_t$ are nodes (grid cells) and $E_s, E_t$ are edges (spatial adjacency). Each node $v_i$ is associated with a feature vector $x_i$, including attributes such as LST, building density, and vegetation index.

A GCN (Kipf and Welling, 2017) extracts spatial features, with embeddings computed as:

$$H^{(l+1)} = \sigma\left(\hat{A}H^{(l)}W^{(l)}\right), \tag{1}$$

where $H^{(l)}$ is the node embedding matrix at layer $l$, $\hat{A} = D^{-1/2}(A + I)D^{-1/2}$ is the normalised adjacency matrix with self-loops, $W^{(l)}$ is the learnable weight matrix, and $\sigma$ is a non-linear activation function.

To align source and target embeddings, a domain discriminator $D$ predicts whether an embedding originates from the source or target domain. A customised Gradient Reversal Layer (GRL) reverses gradients during backpropagation, enforcing domain-invariant embeddings. Specifically, a spatial similarity matrix $S$ is introduced, where $S_{ij}$ quantifies the similarity (i.e., mean proportions of urban features within the corresponding areas of the two cities) between node $i$ in the source graph and node $j$ in the target graph. By prioritising the alignment of regions in the source and target domains that are spatially comparable, the robustness of the feature alignment process is enhanced. Hence, the domain adaptation loss is:

$$\mathcal{L}_{\text{domain}} = -\sum_{i \in V_s} \sum_{j \in V_t} S_{ij} \left[ y_i \log D(h_i) + (1 - y_i) \log(1 - D(h_i)) \right], \tag{2}$$

where $S_{ij}$ is the spatial similarity weight, $h_i$ the embedding of node $i$, and $y_i$ the domain label ($y_i = 0$ for source and $y_i = 1$ for target).

For target predictions, the loss is handled differently as in Equation (3):

- If the source and target cities share similar climates, pseudo-LST values are generated for the target city using the source-trained model. These pseudo-labels are used to supervise the target city's LST prediction.
- If the source and target cities have distinct climates, a small portion (10%) of the target city's labelled data is incorporated to directly supervise the training.

$$\mathcal{L}_{\text{target}} = \begin{cases} \frac{1}{|V_t|} \sum_{i \in V_t} \left( \hat{y}_i - y_i^{\text{pseudo}} \right)^2, & \text{pseudo-labelling} \\ \frac{1}{|V_t^{\text{supervised}}|} \sum_{i \in V_t^{\text{supervised}}} \left( \hat{y}_i - y_i \right)^2, & \text{semi-supervised} \end{cases} \tag{3}$$

where $\hat{y}_i$ is the predicted LST, $y_i^{\text{pseudo}}$ the pseudo-LST label, and $y_i$ the ground truth.

The overall loss is:

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{source}} + \lambda_1 \mathcal{L}_{\text{domain}} + \lambda_2 \mathcal{L}_{\text{target}}, \tag{4}$$

where $\mathcal{L}_{\text{source}}$ is the source prediction loss, and $\lambda_1, \lambda_2$ balance domain adaptation and target objectives. Here, we set the default value of 1 to both $\lambda_1$ and $\lambda_2$.

In line with standard practices for regression models, we used $R^2$ and the Root Mean Squared Error (RMSE) to assess model performance.

### 2.3 Study Areas

The framework was evaluated using Singapore as the source city and Malacca, Melbourne, and Bristol as target cities. Singapore's tropical climate, dense urban morphology, and extensive green spaces serve as the training foundation. Malacca, with its tropical climate and moderate density, tested adaptation to similar domains, while Melbourne and Bristol, temperate cities with significant climatic differences, evaluated the framework's ability to handle diverse environments.

Urban morphology data, including building footprints and road networks, were sourced from OpenStreetMap. Environmental data, such as LST and Normalised Difference Vegetation Index (NDVI), were retrieved from Landsat 8 via Google Earth Engine. LST and NDVI for Singapore and Malacca were retrieved using annual mean values due to their consistent urban heat conditions. Summer LST and NDVI data were retrieved for Bristol from 1 June to 31 August 2020 and for Melbourne from 1 January to 29 February 2020. Population density data came from Meta's Data for Good project (Meta, 2024). Data were harmonised to $1000 \times 1000$-meter resolution defined in Section 2.1 to align with the spatial framework.

## 3 Deal with Spatial Heterogeneity

The results, presented in Figure 2, highlight both the strengths and limitations of the framework in addressing cross-city spatial heterogeneity, supported by statistical evidence that demonstrates its robustness and predictive capability. To evaluate the effectiveness of the two target loss functions proposed in Equation (3), both pseudo-labelling and semi-supervised training approaches were applied to all four cities, allowing for a comparison of their utility across diverse urban settings.

The framework achieved reasonable results in Malacca, which shares a tropical climate and similar urban morphology (road and building densities) with Singapore. Both pseudo-labelled and semi-supervised training approaches yielded high $R^2$ values and low Root Mean Square Error (RMSE), highlighting the framework's robustness when the source and target domains share comparable environmental and morphological characteristics.

In Melbourne and Bristol, where urban morphology and temperate climates differ significantly from Singapore, the GNN-DA framework demonstrated strong performance, achieving reasonable $R^2$ values and low RMSE. Melbourne outperformed Bristol, likely due to its higher summer temperatures, which align more closely with Singapore's tropical climate, facilitating better domain adaptation. These results underscore the framework's robustness in generalising across cities with contrasting climatic and urban characteristics for summertime LST predictions.

Residual maps in Figure 2 reveal the spatial distribution of prediction errors. While GNN-DA reduces domain discrepancies and captures broad spatial trends, it struggles to fully model underlying spatial complexities and microclimatic variations, consistent with geographic principles (Tobler, 2004, 1970).

## 4 Conclusion

This study highlights the potential of the GNN-DA framework to address cross-city spatial heterogeneity in urban heat prediction. By leveraging graph-based representations and domain adaptation techniques, the framework demonstrated strong generalisability across diverse urban environments, particularly under summertime conditions. The successful predictions in Melbourne and Bristol during the summer underscore the framework's ability to transfer critical spatial features across distinct climatic and urban settings, making it a promising tool for addressing global urban heat challenges.

However, the current implementation is trained on a single summer season, which may not fully capture inter-annual variability or longer-term non-stationary trends associated with future climate change. Future work will therefore examine whether incorporating multi-year observations improves model robustness under evolving urban heat regimes. In addition, while the framework performs well in relatively warm urban contexts, its transferability to cities characterised by colder and/or drier climates remains to be evaluated through expanded cross-city training.

Nevertheless, the findings emphasise the importance of balancing local specificity with cross-domain generalisation in GeoAI-based urban climate modelling, highlighting the promise of GNN-DA as

| Cross-City Comparisons | Malacca | | Melbourne (Central Urban Area) | | Bristol | |
|---|---|---|---|---|---|---|
| | $R^2$ | RMSE | $R^2$ | RMSE | $R^2$ | RMSE |
| CNN-DA (pseudo-labelling) | 0.69 | 1.92 | 0.66 | 0.56 | 0.44 | 2.17 |
| CNN-DA (semi-supervised) | 0.73 | 1.06 | 0.71 | 0.48 | 0.51 | 1.41 |
| Random Forest | 0.15 | 4.03 | 0.00 | 3.68 | 0.00 | 5.01 |

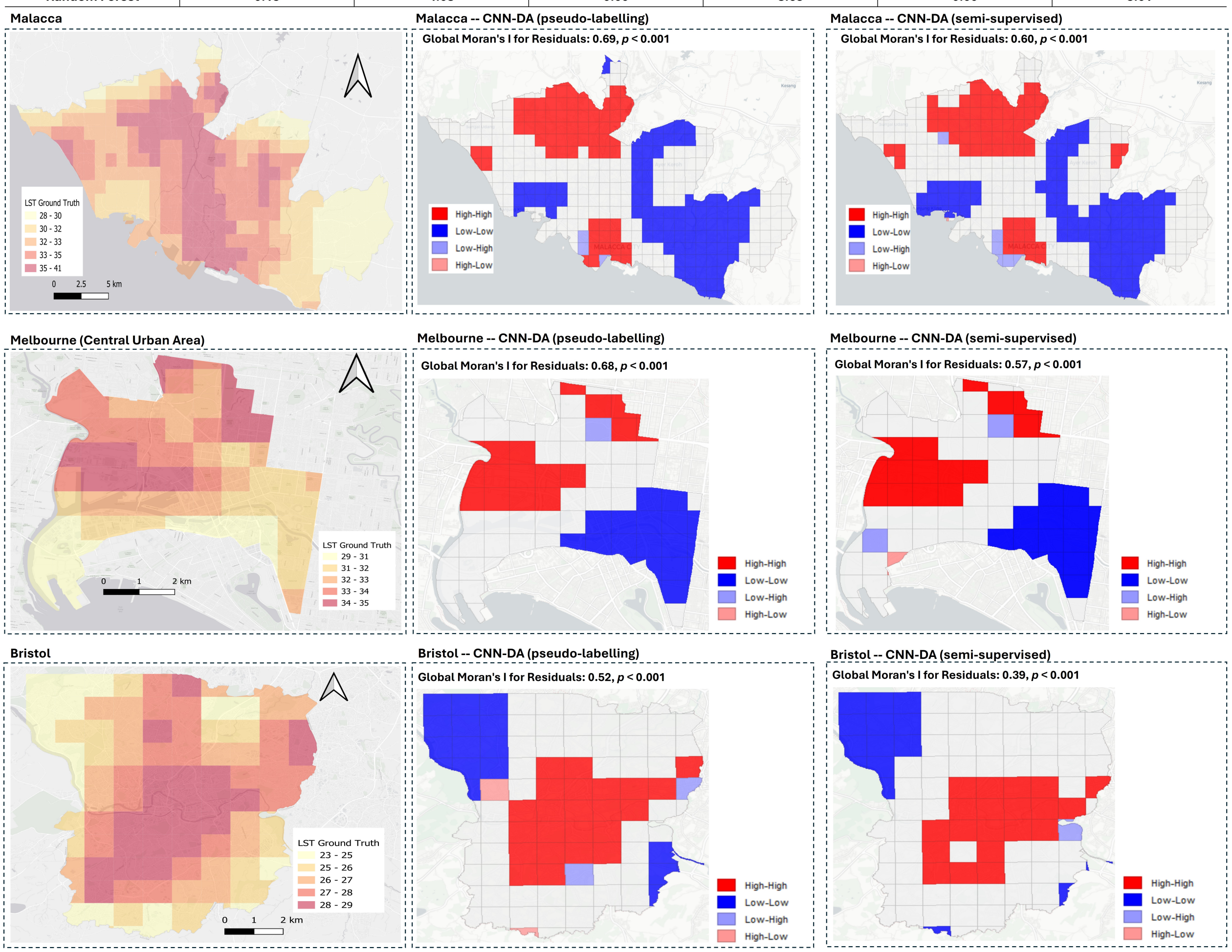


Figure 2: Cross-city Comparisons for summertime LST predictions.

a scalable approach for supporting climate-resilient urban planning across heterogeneous urban systems.

## 5 Acknowledgements

The research was conducted at the Future Cities Lab Global at the Singapore-ETH Centre, established collaboratively between ETH Zurich and the National Research Foundation Singapore. This research is supported by the National Research Foundation Singapore (NRF) under its Campus for Research Excellence and Technological Enterprise (CREATE) programme.

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