GNNWR: An Open-Source Package of Spatiotemporal Intelligent Regression Methods for Modeling Spatial and Temporal Non-Stationarity

Ziyu Yin[1,*], Jiale Ding[1,*], Yi Liu[1], Ruoxu Wang[1], Yige Wang[1], Yijun Chen[1], Jin Qi[1], Sensen Wu[1], and Zhenhong Du[1]

[1]Zhejiang University, School of Earth Sciences
[*]These authors contributed equally to this work.

Correspondence: Sensen Wu (wesensengis@zju.edu.cn)

Abstract. Spatiotemporal regression is a crucial method in geography for discerning spatiotemporal non-stationarity in geographical relationships, which has found widespread application across diverse research domains. This study implements two innovative spatiotemporal intelligent regression models, namely ~~geographically neural network weighted regression~~ Geographically Neural Network Weighted Regression (GNNWR) and ~~geographically and temporally neural network weighted regression~~ Geographically and Temporally Neural Network Weighted Regression (GTNNWR), ~~integrating the spatiotemporal weighted framework and neural networks . Demonstrating superior~~ which using neural networks to estimate the spatiotemporal non-stationarity. Due to the higher accuracy and generalization ~~capabilities in large-scale data environments compared to traditional methods~~ability, these models have ~~emerged as prominent tools~~been widely used in various fields of scientific research. To facilitate the ~~seamless~~ application of GNNWR and GTNNWR in addressing spatiotemporal non-stationary processes, a Python-based package, GNNWR, has been developed. This article details the implementation of these models and introduces the GNNWR package, enabling users to efficiently apply these cutting-edge techniques. Validation of the package is conducted through two case studies. The first case involves the verification of GNNWR using air quality data from China, while the second employs offshore dissolved silicate concentration data from Zhejiang Province to validate GTNNWR. The results of the case studies underscore the effectiveness of the GNNWR package, yielding outcomes of notable accuracy. This contribution anticipates a significant role for the developed package in supporting future research that leverages big data and spatiotemporal regression techniques.

1 Introduction

Spatiotemporal non-stationarity, denoting variations in geographical elements or structures across different temporal and spatial contexts, constitutes an intrinsic attribute of nearly all kinds of geographical processes and phenomena. Geographically Weighted Regression (GWR), a classic methodology for delineating spatial non-stationarity in geographical relationships, facilitates the variations of parameter coefficients within the regression equation according to

spatial locations (Brunsdon et al., 1996). As a foundational algorithm within the domain of spatiotemporal regression analysis, GWR has been widely used across diverse research domains, including environmental studies (Yang et al.,
25 2019; Shen et al., 2023), urban studies (Sisman and Aydinoglu, 2022; He et al., 2023), and the social sciences (Stein et al., 2015; Lewandowska-Gwarda, 2018; Ahadnejad Reveshty et al., 2023).

On the basis of GWR, various methods have been proposed that focus on optimizing the model ability to solve spatiotemporal non-stationary relationships. The improvements mainly include the following aspects: the selection of spatiotemporal distance metrics (Fotheringham et al., 2015; Lu et al., 2014), the choice of weight kernel func-
30 tions (Fotheringham et al., 2017), and the optimization of statistical diagnostic methods (Brunsdon et al., 1999; Leung et al., 2000). Notably, multi-scale geographically weighted regression (MGWR) extends the weight kernel function to possess varying bandwidths for each independent variable and further enhances the model capacity to fit spatial non-stationarity (Fotheringham et al., 2017). To deploy the MGWR model, researchers developed a Python-based ~~(van Rossum, 2011) software package MGWR~~ software package `mgwr` that focuses on multi-scale estimation
35 and efficient computation of spatial non-stationarity (Oshan et al., 2019). It supplements the R-language-based ~~(Team, 2017)~~ open-source tools~~(e.g., spgwr (Bivand and Yu, 2023), gwrr~~, e.g., `spgwr` (Bivand and Yu, 2023), `gwrr` (Wheeler, 2022), and ~~GWmodel (Lu et al., 2024))~~`GWmodel` (Lu et al., 2024), improving the overall accessibility of GWR and MGWR methods.

Owing to the intricate linear interplay between spatial distance and non-stationary weights inherent in geograph-
40 ical processes, the precise computation of the weight matrix through simple kernel functions encounters notable challenges. In response to this, diverse methodologies within the domain of geospatial artificial intelligence (GeoAI) have been proposed to effectively capture the non-linear spatial relationships among pertinent factors (Georganos and Kalogirou, 2022; Hagenauer and Helbich, 2022). The majority of existing GeoAI approaches utilize neural networks in an opaque manner for establishing spatial relationships, leading to a constrained spatial interpretability of the
45 estimated relationships. To address this, researchers have integrated a spatiotemporal weighted framework with neural networks, leading to the formulation of spatiotemporal intelligent regression models. Notably, the ~~geographically neural network weighted~~ Geographically Neural Network Weighted regression (GNNWR) model has been introduced, which employs neural networks to learn the non-linear relationship between spatial distance and non-stationary weights (Du et al., 2020a). Taking inspiration from GWR, GNNWR employs a ~~spatially weighted neural network~~
50 Spatially Weighted Neural Network (SWNN) to accurately derive the spatial weight matrix. Subsequently, this SWNN is combined with an ordinary linear regression (OLR) model to estimate spatial non-stationarity.

In addition to space, time is another fundamental dimension associated with geographical processes. In recent years, numerous studies have focused on incorporating temporal effects into GWR model to account for both temporal and spatial non-stationarity (Huang et al., 2010; Fotheringham et al., 2015). Recognizing that time and space exhibit
55 distinct scale effects, Huang et al. (2010) proposed a straightforward approach to combine spatial and temporal distances into a unified space-time distance, leading to the development of the ~~geographically and temporally weighted regression~~ Geographically and Temporally Weighted Regression (GTWR) model. The GTWR model, along with its

extended methodologies, has been effectively applied across various domains, producing remarkable results and offering satisfactory interpretability (Ma et al., 2018; He and Huang, 2018; Guo et al., 2021; Wang et al., 2022).

60 However, the form of space-time distance usually requires a priori assumption and should be assumed to be relatively simple (e.g., linear weighted function) so as to eliminate the estimation problem in the terminal model. Considering that neural networks have the potential to capture the complex non-linear effects in space-time, Wu et al. (2021) proposed a ~~spatiotemporal proximity neural network~~ SpatioTemporal Proximity Neural Network (STPNN) to accurately generate space-time distance and extended GNNWR with the STPNN to incorporate temporal effects into

65 spatial non-stationarity. Accordingly, a spatiotemporal intelligent regression model named geographically and temporally neural network weighted regression (GTNNWR) was developed to estimate spatiotemporal non-stationary relationships.

In recent years, GNNWR and GTNNWR have been widely applied in various fields and have achieved excellent fitting capabilities and geographical interpretability, such as atmospheric pollution (Chen et al., 2021; Ni et al., 2022; Liu

70 et al., 2023), environmental modeling ~~(?Du et al., 2021; Wu et al., 2022; Qi et al., 2023)~~ (Wu et al., 2019; Du et al., 2021; Wu et al.) and urban geography (Wang et al., 2022; Yang et al., 2022; Liang et al., 2023). ~~To date, there has been a notable absence of dedicated software pertaining specifically to the GNNWR and GTNNWR models. To~~ However, the accessible version for the source code of GNNWR (Du, 2019) and GTNNWR (Wu, 2020) are implemented with TensorFlow 1.x, which is too old to run in the latest hardware environment. And the codes are not highly encapsulated,

75 which makes researchers harder to use and develop the model. Therefore, there is a need to develop a set of model implementations with a newer architecture, simpler usage, and clearer code structure to facilitate the utilization of these spatiotemporal intelligent regression models by researchers ~~across diverse domains~~ in different fields, and to solicit ~~feedback~~ feedbacks for refinement and enhancement of ~~the models, we have introduced~~ these models.

This research has developed an open-source Python package, denoted as the ~~GNNWR package. This package~~

80 ~~is designed~~ `GNNWR` package, to furnish a suite of spatiotemporal intelligent regression models, encompassing the GNNWR and GTNNWR variants, thereby serving as a resource for researchers seeking to address challenges within their respective fields.

The GNNWR package offers a comprehensive workflow analysis capability, enabling users to create datasets, instantiate models, conduct training, and generate output results, as well as perform model predictions and visual-

85 izations. The GNNWR package uses PyTorch as a deep learning framework ~~(?)~~ (Paszke et al., 2019), and its dynamic computational graph makes model construction and debugging more intuitive. This package provides extended models as well as great flexibility, allowing advanced users to design custom models based on existing models using the PyTorch framework.

The remainder of this article is constructed as follows. In Section 2, we provide an review for the GNNWR and

90 GTNNWR model that the package has implemented; in Section 3, we describe the package architecture and offer usage example for the package; finally, in section 4, we conclude a summary of our outcomes and suggests potential avenues for future development.

2   Model Review

This section offers a concise overview of the GNNWR family of models, which are accommodated by the GNNWR

95 package. ~~The regression~~ Detailed descriptions and performance analysis can be referred to the original articles (Du et al., 2020a; Wu et al., 2021).

2.1   OLR and GWR

For a regression relation with p independent variables and n observations, the regression formula of the classic ~~OLR~~ Ordinary Least squares Regression (OLR) model is expressed as:

100
$$y_i = \beta^{OLR}{}_0 + \sum_{k=1}^{p} \beta^{OLR}{}_k x_{ik} + \varepsilon_i \quad \text{for } i = 1, 2, \ldots, n \tag{1}$$

where y_i and ~~$x_{i1}, x_{i2}, \ldots, x_{ip}$~~ x_{ik} are the dependent variable and ~~independent variables; $\beta_0, \beta_1, \ldots, \beta_p$ are the regressive coefficients, and~~ k-th independent variable at observation i; β_k^{OLR} is the regressive coefficient for the k-th independent variable and β_0^{OLR} is the intercept term; ε_i is the error term. ~~The~~

Considering the spatial non-stationarity, the GWR model extends OLR approach to enable spatially localized

105 estimates, ~~the formula is~~ by allowing local variations in rates of change. Thus, regression can be represented as:

$$y_i = \beta_0(u_i, v_i) + \sum_{k=1}^{p} \beta_k(u_i, v_i) x_{ik} + \epsilon_i \quad \text{for } i = 1, 2, \ldots, n \tag{2}$$

~~Based on the geographically weighted idea similar to GWR, the GNNWR model considers the spatial non-stationarity of the regression relationship as the fluctuation change as the fluctuation change at different locations on the OLR levels (Du et al., 2020a). In the GNNWR model, the spatial non-stationarity can be represented as:~~ where $\beta_0(u_i, v_i)$

110 and $\beta_k(u_i, v_i)$ are the localized regression coefficient for the constant term and the k-th independent variable at location (u_i, v_i). Their estimation can be calculated with a weighted least squares method:

$$y_i = w_0 \hat{\boldsymbol{\beta}}(u_i, v_i) \times \beta_0^{OLR} + \sum_{k=1}^{p} w_k = (\mathbf{X}^\top \mathbf{W}(u_i, \ v_i) \times \beta_k^{OLR} x_{ik} + \epsilon \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{W}(u_i \ \text{for } i = 1, 2, \ldots, n\, v_i) \mathbf{y} \tag{3}$$

where ~~$w_k(u_i, v_i)$ represents the non-stationary weight of the OLR coefficient β_k^{OLR}. Therefore, the calculation formula for $\hat{y}_i$ is:~~

115
$$\hat{y}_i = \sum_{k=0}^{p} \hat{\beta}_k(u_i, v_i) x_{ik} = \sum_{k=0}^{p} w_k(u_i, v_i) \times \hat{\beta}_{k\mathrm{OLR}} x_{ik}$$

~~The modeling capability of GWR for geographical relationships depends on the fitting and solving ability of the weight kernel function for spatial non-stationarity. The kernelfunctions of GWR can be abstracted as follows:~~

$\mathbf{W}(u_i, v_i)$ is the spatial weighting diagonal matrix at fit point i, $\mathbf{y}$ and $\mathbf{X}$ are the dependent and independent variables for all the observations. A distance-decaying kernel function (e.g. Gaussian kernel) is then employed to calculate the spatial weights from the fit point to its neighboring observations within the bandwidth b:

$$w_{ij} = f_{\text{kernel}}(d_{ij}, b)\exp[-(d_{ij}/b)^2] \tag{4}$$

~~Where d_{ij} represents~~ where d_{ij} is the distance between ~~samples, and b represents the bandwidth~~fit point i and its neighbor j.

~~To accurately fit the complexrelationship between spatial proximity and non-stationary weights, the GNNWR model designed a SWNN to realize the neural network expression of the weight kernel function.~~

2.2 GNNWR

Since a pre-defined kernel function might not accurately estimate the complex, heterogenous geographical processes. The GNNWR model introduces a spatially weighted neural network (SWNN) to represent the nonstationary weight matrix (Figure 1).

The spatial weight estimation for point ~~i~~i is calculated as follows:

$$\underline{W_i = W}\mathbf{W}(u_i, v_i) = \underline{SWNN}\text{SWNN}([d_{i1}^S, d_{i2}^S, \ldots, d_{in}^S]^{\underline{T}\top}) \tag{5}$$

where $[d_{i1}^S, d_{i2}^S, \ldots, d_{in}^S]$ is the distances from location i to ~~training samples.~~ other training samples, and the weighting matrix $\mathbf{W}(u_i, v_i)$ is a diagonal matrix, whose diagnostic elements are the non-stationary weights $w_0(u_i, v_i), w_1(u_i, v_i), \ldots, w_p(u_i, v_i)$ for the regression.

Accordingly, GNNWR model describes spatial non-stationarity through fluctuating changes in the coefficients of OLR at different locations (Du et al., 2020a). Thereby the spatial non-stationarity can be represented as:

$$y_i = w_0(u_i, v_i)\beta_0^{OLR} + \sum_{k=1}^{p} w_k(u_i, v_i)\beta_k^{OLR} x_{ik} + \epsilon_i \quad \text{for } i = 1, 2, \ldots, n. \tag{6}$$

Then, the estimates of dependent variable in GNNWR can be calculated as:

$$\hat{\boldsymbol{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{x_1}^\top \mathbf{W}(u_1, v_1)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \\ \boldsymbol{x_2}^\top \mathbf{W}(u_2, v_2)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \\ \vdots \\ \boldsymbol{x_n}^\top \mathbf{W}(u_n, v_n)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \end{bmatrix} \boldsymbol{y} = \begin{bmatrix} \boldsymbol{x_1}^\top \text{SWNN}([d_{i1}^S, d_{i2}^S, \ldots, d_{in}^S]^\top)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \\ \boldsymbol{x_2}^\top \text{SWNN}([d_{i1}^S, d_{i2}^S, \ldots, d_{in}^S]^\top)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \\ \vdots \\ \boldsymbol{x_n}^\top \text{SWNN}([d_{i1}^S, d_{i2}^S, \ldots, d_{in}^S]^\top)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \end{bmatrix} \boldsymbol{y} = \boldsymbol{Sy} \tag{7}$$

where $\boldsymbol{S}$ is the hat matrix of the GNNWR model.

2.3 GTNNWR

Alongside space, time constitutes a fundamental dimension in the study of geographic phenomena. The GTNNWR model extends the spatial form of the non-stationary relationship in Eq. ~~(??)~~(6) to the following spatiotemporal
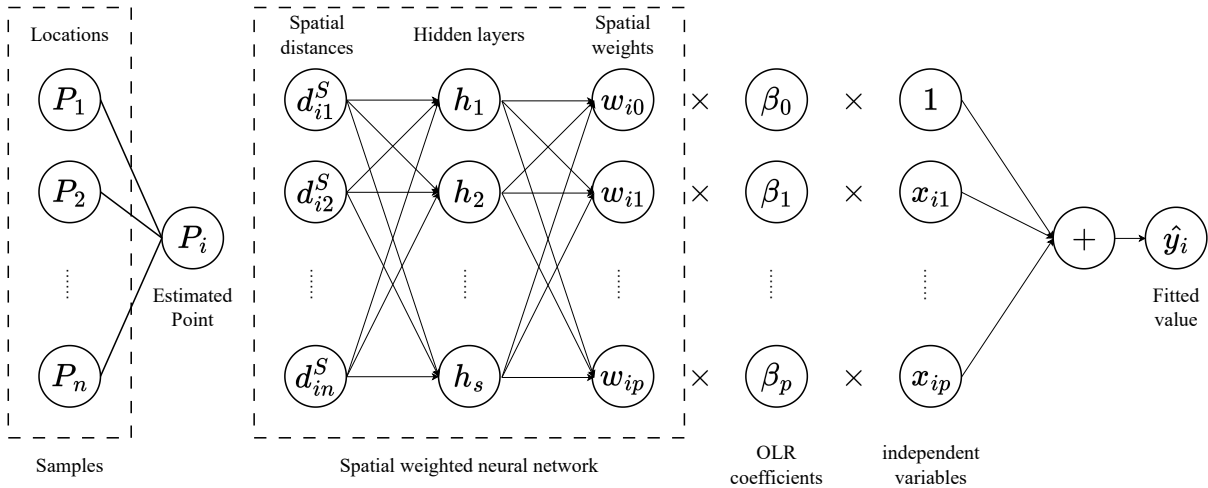
Figure 1. The framework of the GNNWR model.

form:

$$y_i = \beta_0(u_i, v_i, t_i) + \sum_{k=1}^{p} \beta_k(u_i, v_i, t_i)x_{ik} + \varepsilon_i, \quad \text{for } i = 1, 2, \ldots, n$$

145

$$= w_0(u_i, v_i, t_i)\beta_0^{OLR} + \sum_{k=1}^{p} w_k(u_i, v_i, t_i)\beta_k^{OLR}x_{ik} + \varepsilon_i, \quad \text{for } i = 1, 2, \ldots, n$$

(8)

where $w_k(u_i, v_i, t_i)$ represents the spatiotemporal non-stationary weight of β_k^{OLR}, which is determined by its spatiotemporal location (u_i, v_i, t_i) and influenced by other samples.

Similar to the SWNN of GNNWR, the GTNNWR model ~~,as shown in figure 2,~~ designed a spatiotemporal weighted neural network (STWNN) calculate the spatiotemporal weights as follows:

150

$$\underline{W}\boldsymbol{W}(u_i, v_i, t_i) = \text{STWNN}\left(\left[d_{i1}^{ST}, d_{i2}^{ST}, \ldots, d_{in}^{ST}\right] \underline{{}^{T}}{}^{\top}\right)$$

(9)

where $\left[d_{i1}^{ST}, d_{i2}^{ST}, \ldots, d_{in}^{ST}\right]$ are the spatiotemporal distances from point i to other training samples. This expression indicates that the spatiotemporal non-stationary weight is determined by the spatiotemporal distance. To quantify the spatiotemporal distance, Huang et al. (2010) defined the distance as the following form:

$$d_{ij}^{ST} = d_{ij}^{S} \otimes d_{ij}^{T}$$

(10)

155   where ~~d_{ij}^{S}, d_{ij}^{T}, and d_{ij}^{ST} respectively denote the spatial distance, temporal distance, and spatiotemporal distance , and the symbol $\otimes$ represents the operator.~~ symbol $\otimes$ represents a fusion operator which integrates temporal (d_{ij}^{T}) and spatial (d_{ij}^{S}) distance into a spatiotemporal distance d_{ij}^{ST}.

To fully capture the nonlinear effects in ~~spatiotemporal~~the spatiotemporal dimension, Wu et al. (2021) proposed ~~an spatiotemporal proximity neural network(STPNN) based on the spatial distance d_{ij}^{S} and temporal distance d_{ij}^{T}~~

$$d_{ij}^{ST} = \text{STPNN}\left(d_{ij}^S, d_{ij}^T\right)$$

where d_{ij}^{ST} is a vector that indicates the spatiotemporal proximity between points i and j. Therefore, Equation (5) can be refined as:

$$W(u_i, v_i, t_i) = \text{STWNN}\left(\left[d_{i1}^{ST}, d_{i2}^{ST}, \ldots, d_{in}^{ST}\right]^T\right)$$
$$= \text{STWNN}\left(\left[\text{STPNN}\left(d_{i1}^S, d_{i1}^T\right), \ldots, \text{STPNN}\left(d_{in}^S, d_{in}^T\right)\right]^T\right)$$

Therefore, the spatialtemporal the STPNN as the fusion operator $\otimes$. Therefore, the spatiotemporal weight matrix for any given point across time and space can be derived by merging the STPNN with the STWNN through Eq. (??) (Figure 2). Through integrating :

$$\boldsymbol{W}(u_i, v_i, t_i) = \text{STWNN}\left(\left[d_{i1}^{ST}, d_{i2}^{ST}, \ldots, d_{in}^{ST}\right]^T\right)$$
$$= \text{STWNN}\left(\left[\text{STPNN}\left(d_{i1}^S, d_{i1}^T\right), \ldots, \text{STPNN}\left(d_{in}^S, d_{in}^T\right)\right]^T\right). \tag{11}$$

The spatiotemporal weights are then integrated with global OLR estimatesand the , generating continuous space-time weight matrix, the continuous spatial-temporal variable coefficientsis attained. Just like the GTWR model, we can use these coefficients to explain the estimated relationship and make spatiotemporal inference. Hence, the fitted values $\hat{y} = (\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n)$ are computed varying coefficients, and the regression relationship of GTNNWR can be expressed as:

$$y_i = w_0(u_i, v_i, t_i)\beta_0^{OLR} + \sum_{k=1}^{p} w_k(u_i, v_i, t_i)\beta_k^{OLR} x_{ik} + \epsilon_i \quad \text{for } i = 1, 2, \ldots, n \tag{12}$$

where $w_k(u_i, v_i, t_i)$ are the diagonal elements of the spatiotemporal weight matrix $\boldsymbol{W}(u_i, v_i, t_i)$.
And the estimated dependent variables $\hat{y}$ can be calculated as:

$$\hat{\boldsymbol{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{x_1}^\top \boldsymbol{W}(u_1, v_1, t_1)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \\ \boldsymbol{x_2}^\top \boldsymbol{W}(u_2, v_2, t_2)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \\ \vdots \\ \boldsymbol{x_n}^\top \boldsymbol{W}(u_n, v_n, t_n)(\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \end{bmatrix} \boldsymbol{y} = \boldsymbol{S}\boldsymbol{y} \tag{13}$$

where S where $\boldsymbol{S}$ is the hat matrix of the GTNNWR model.

3 Usage ExamplePackage Descriptions

In this section, we present a comprehensive overview of the GNNWR package `gnnwr` package (version 0.1.11) and the range of models it supports. We begin by introducing the fundamental architecture of the software package,
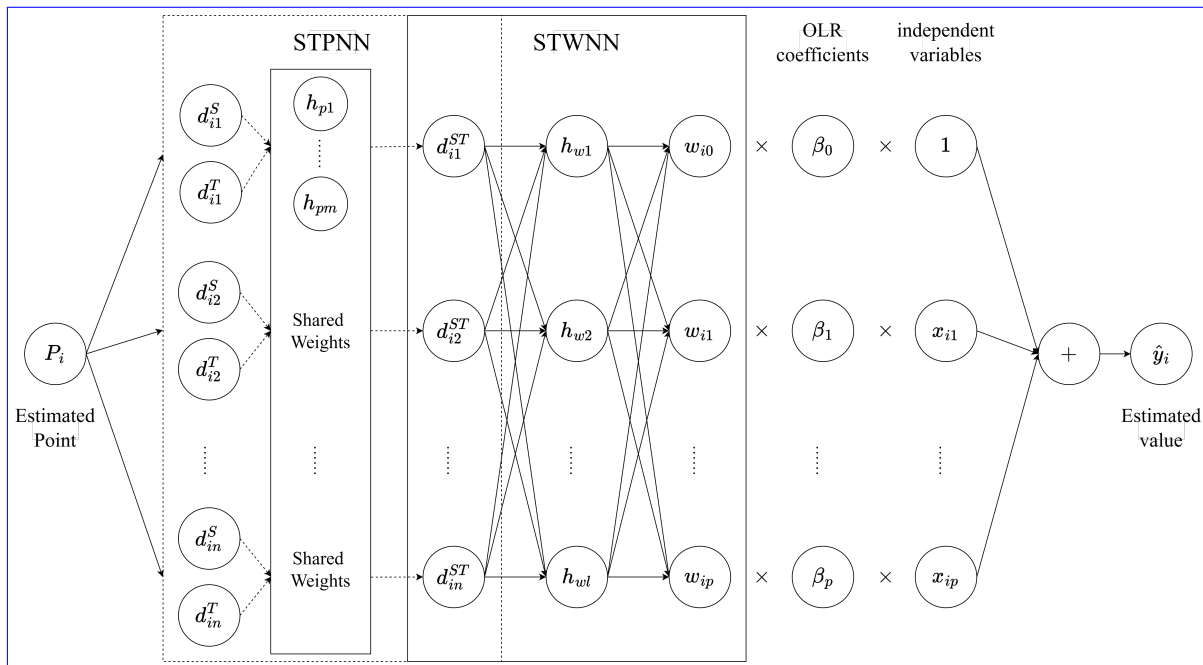
Figure 2. The framework of the GTNNWR model. d_{ij}^S and d_{ij}^T represent the spatial distance and temporal distance between the estimated points P_i and P_j, respectively. The spatiotemporal proximity d_{ij}^{ST} is obtained by integrating d_{ij}^S and d_{ij}^T through the STPNN.

delving into its essential components and functionalities. Following this, we outline the analysis process employed in utilizing the package, showcasing its practical application through two case studies.

3.1 Package Architecture

185   The ~~GNNWR~~ gnnwr package is designed with a modular architecture, enabling the integration of diverse module strategies to facilitate a variety of task workflows. It comprises four primary modules: `Dataset`, `Network`, `Utils`, and `Model`.

3.1.1 Dataset

The `Dataset` module specifies the data types employed throughout the package. It includes the `BasicDataset`
190   class for training and the `PredictDataset` class for prediction. This module also offers preprocessing functions that convert Pandas' `DataFrame` data into the necessary formats (McKinney et al., 2010), handling tasks such as normalization and dataset partitioning. Additionally, it provides methods for saving and loading datasets, enabling users to directly work with processed data files and instantiate data objects.

3.1.2 `Network`

The `Network` module, extending PyTorch's `nn.Module` class, defines the architectures for models such as `SWNN` and `STPNN`. It allows users with programming expertise to customize new network structures based on existing ones, adapting to their specific research requirements.

3.1.3 `Utils`

The `Utils` module contains classes for statistical diagnostics and visualization techniques specific to spatial weighted regression. These diagnostic classes offer a suite of methods to evaluate model performance, while the visualization classes employ map-based representations to enhance the analysis of spatial data and model outcomes.

3.1.4 `Model`

The `Model` module is the cornerstone of the package, providing two classes: `GNNWR` and `GTNNWR`. `GNNWR` acts as the foundational class, with `GTNNWR` being its subclass. These classes encapsulate methods for model training, prediction, diagnostics, and loading. Users can easily invoke these methods to employ the models for problem analysis and forecasting on unseen data.
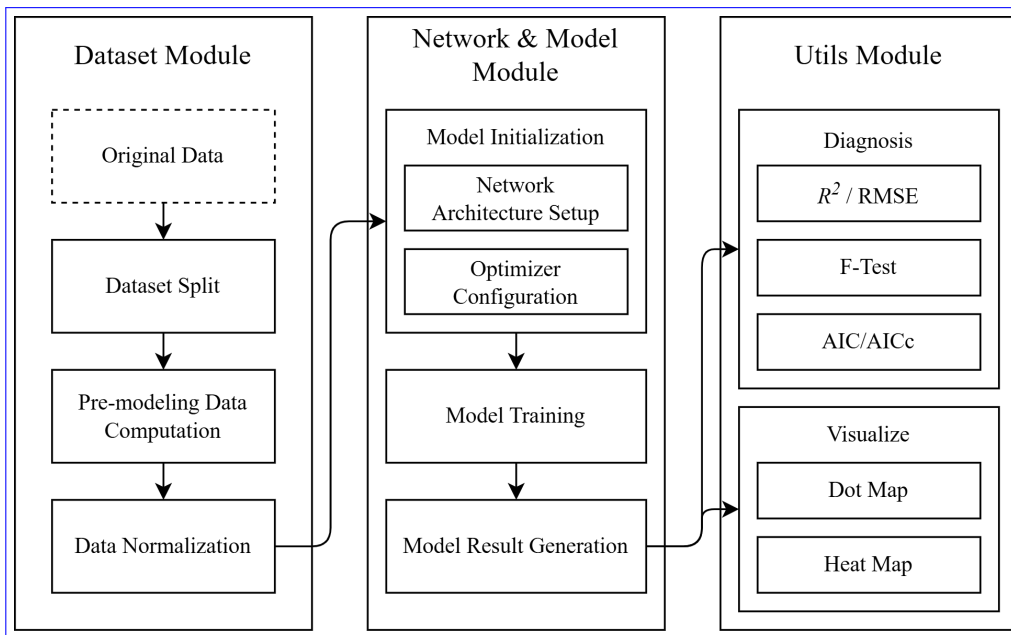
Figure 3. Workflow diagram of the package. Dashed boxes denote the raw data, solid boxes represent the code process modules, and arrows indicate the direction of data flow.

3.2 Usage Example for GNNWR

We commence our investigation by examining air quality modeling through the analysis of data gathered from Chinese air monitoring stations (Du et al., 2020b). This analysis seeks to delineate the spatially non-stationary associations between PM2.5 (particulate matter with aerodynamic diameter less than 2.5 μm) concentrations and their environmental determinants. Given the pivotal role of PM2.5 as an indicator of air quality, elucidating its spatial variability is crucial for comprehending the underlying spatial processes and environmental dynamics of atmospheric contamination (Han et al., 2016). The objective of this study is to develop a predictive model for the annual average PM2.5 concentrations in the study area at a 3 km x 3 km spatial resolution for the year 2017. The model incorporates meteorological variables such as Aerosol Optical Depth (AOD), temperature (TEMP), precipitation (TP), wind speed (WS), and wind direction (WD), along with elevation data (DEM).

3.2.1 Dataset initialization

Upon loading the dataset as a Pandas' `DataFrame`, the `init_dataset` function from the GNNWR package is utilized to convert it into a suitable format for model input. This function ~~proportionally allocates~~ randomly divides the dataset into training, validation ~~, and test subsets~~, and testing subsets according to the ratio specified in the input parameters; and computes the distance vectors for each sample, which are crucial for both model training and performance evaluation. In this specific experiment, 15% of the data is allocated to the testing set; and out of the remaining 85%, 10% was used as validation set and the rest as training set.

In this context, it is essential to specify the independent variables, dependent variables, and spatial position variables, which correspond to the `x_column`, `y_column`, and `spatial_column` parameters of the `init_dataset` function, respectively.

When calculating the distance, the `init_dataset` function, by default, uses Euclidean distance to compute the spatial distances between feature points. This process generates a spatial distance vector for each point, which serves as input to the neural network component of the model. To accommodate various research requirements, the `spatial_fun` parameter enables users to provide a custom method for calculating spatial distances.

To optimize the speed of model training and enhance the precision of model outcomes, the function preprocesses the independent and dependent variables by default. It typically employs normalization for preprocessing; however, users have the option to adjust the `process_fun` parameter to utilize standardization instead.

```
1: >>> from gnnwr.datasets import init_dataset
2: >>> train_set, val_set, test_set = init_dataset(data=data,
3: ...                                      test_ratio=0.2,
4: ...                                      valid_ratio=0.2,
5: ...                                      test_ratio=0.15,
6: ...                                      valid_ratio=0.1,
```

```
7: ...                                              x_column=x_column,
8: ...                                              y_column=y_column,
9: ...                                              spatial_column=spatial_column)
```

3.2.2 Model configuration and running

To continue, we need to create an instance of the GNNWR model. After importing the `gnnwr.models` module, we can do so by invoking the GNNWR class. The `dense_layers` parameter allows us to specify the number of hidden layers in the model's neural network, with each layer consisting of a fully connected layer, a batch normalization layer, a dropout layer, and an activation function. These hyperparameters are closely linked to the neural network's architecture, encompassing aspects such as the use of a batch normalization layer, the dropout rate, and the activation function's type, among others. In this specific example, we have configured a neural network with a hidden layer that includes three sub-layers, each with 1024, 512, 256, and 128 nodes, respectively. The activation function uses a ~~PReLU~~ Parametric Rectified Linear Unit (PReLU) function with an initial value of ~~0.1~~0.2, while all other settings are kept at their default values.

The GNNWR class uses Adadelta as its default optimizer, with an initial learning rate of ~~0.2~~0.6, and employs cosine annealing warm restart as its learning rate adjustment strategy. The class also supports a range of optimizers, including Stochastic Gradient Descent (SGD), Adam, Adagrad, RMSprop, and various learning rate adjustment strategies, such as multistep and cosine annealing. These optimizers and strategies contribute to improving the model's training efficiency and performance, thereby enabling it to better accomplish its tasks.

Additionally, GNNWR involves dropout and batch normalization strategies to avoid overfitting and improve generalizability and performance of the model. The default dropout rate is 0.2, and can be altered through the `drop_out` parameter; and the model applies batch normalization by default, which can be disabled by setting the `batch_norm` parameter into `False`.

To streamline model training, we can utilize the `run` function to specify the number of iterations and the frequency of printing training process information, allowing us to monitor the training progress and performance. Throughout the training process, we will retain the best-performing model within the validation set to prevent the GNNWR model from overfitting. Selecting the optimal model helps minimize the expected error and guarantees that the model possesses superior generalization ability. For storage convenience, the model repository will only retain a file containing the neural network components of the model. This file encapsulates the structural configuration and parameter information of the neural network.

```
1: >>> from gnnwr import models
2: >>> from torch import nn
3: >>> gnnwr = models.GNNWR(train_dataset = train_set,
4: ...                      valid_dataset = val_set,
```

```
 5: ...                          test_dataset = test_set,
 6: ...                          dense_layers = [1024, 256, 128],
 7: ...                          dense_layers = [1024, 512, 256, 128],
 8: ...                          activate_func = nn.PReLU(init=0.2),
 9: ...                          start_lr = 0.1,
10: ...                          start_lr = 0.6,
11: ...                          optimizer = "Adadelta",
12: ...                          drop_out = 0.2,
13: ...                          batch_norm = True,
14: ...                          model_name = "GNNWR_PM25")
15: >>> gnnwr.run(max_epoch = 4000, print_frequency = 500)
16: >>> gnnwr.run(max_epoch = 2000, print_frequency = 500)
```

The GNNWR package uses Tensorboard to record the model training process, including the loss and R^2 scores on the training and validation sets for each epoch, as well as the learning rate and best R^2 scores obtained on the validation set. By observing the changes in the model during the training process, targeted adjustments to the training method can be made. To enhance users' comprehension of the model architecture, we have incorporated the `add_graph` function. When utilized, this function enables users to visualize the structure of the model within the "Graphs" section of TensorBoard. This functionality not only clarifies the model's architecture but also facilitates the prompt identification of issues during model debugging and optimization, thereby substantially improving model performance.

3.2.3   Result and visualization

We can obtain the composition and results of the model through the `result` method, including the model structure, optimizer structure, used variables, and the accuracy, complexity, and content of statistical tests performed on the model. Among them, the R^2 and RMSE(Root Mean Square Error) indicators summarize the model's fitting ability, while the AIC and AICc indicators provide a deeper understanding of the model's complexity. The F_1, F_2, and F_3 statistical data are used as sample diagnostic measures(?)(Wu et al., 2019). The first two values indicate the presence of significant spatiotemporal non-stationarity in the model, while the last value evaluates the significance of spatiotemporal non-stationarity in the regression parameters of each independent variable.

```
>>> gnnwr.result()
```

```
1: -------------------Model Information-----------------
2: Model Name:            | GNNWR_PM25
3: independent variable:  | ['dem', 'w10', 'd10', 't2m', 'aod_sat', 'tp']
```

```
 4: dependent variable:    | ['PM2_5']
 5:
 6: OLS coefficients:
 7: x0: 7.20676
 8: x1: -7.51571
 9: x2: 0.00989
10: x3: 21.75958
11: x4: 30.29816
12: x5: -26.90607
13: Intercept: 22.79182
14: x0: 7.12861
15: x1: -4.03670
16: x2: -1.90988
17: x3: 21.29951
18: x4: 36.57638
19: x5: -24.50677
20: Intercept: 19.16957
21:
22: -------------------Result Information----------------
23: Test Loss: |                        33.63722
24: Test R2   : |                        0.84065
25: Train R2 : |                         0.82611
26: Valid R2 : |                         0.84560
27: RMSE: |                              5.79976
28: AIC:  |                              1798.68992
29: AICc: |                              1791.50793
30: F1:   |                              0.19219
31: F2:   |                              2.40907
32: f3_param_0: |                        10.68157
33: f3_param_1: |                        1.81385
34: f3_param_2: |                        3.81711
35: f3_param_3: |                        54.19521
36: f3_param_4: |                        382.45236
37: f3_param_5: |                        117.74578
38: f3_param_6: |                        21.48253
```

```
39: Test_Loss: |                         33.42091
40: Test_R2   : |                          0.84280
41: Train_R2 : |                           0.84762
42: Valid_R2 : |                           0.84541
43: RMSE: |                                5.78108
44: AIC:  |                             1257.37056
45: AICc: |                             1254.68787
46: F1:   |                                0.11974
47: F2:   |                                3.52673
48: f3_param_0: |                          1.81630
49: f3_param_1: |                         19.05118
50: f3_param_2: |                          0.42682
51: f3_param_3: |                         68.13538
52: f3_param_4: |                         47.61187
53: f3_param_5: |                        170.05663
54: f3_param_6: |                        122.83797
```

The empirical results reveal that the model exhibits robust performance in the reconstruction of PM2.5 distributions. ~~Notably~~, and the statistical analyses confirm the presence of significant spatial heterogeneity in PM2.5 concentrations. In terms of statistical indicators, the model achieved R^2 scores of ~~0.826~~ 0.848 for the training dataset, ~~0.846~~ 0.845 for the validation dataset, and ~~0.841~~ 0.843 for the test dataset, which are much higher than traditional models like OLS and GWR (implemented with the `mgwr` package by Oshan et al., version 2.2.1). Also, the residuals of GNNWR are generally smaller than those of traditional models, with most residuals being close to zero and rarely showing large deviations (Figure 4). Such outstanding performance reflects GNNWR's capability of capturing complex patterns in spatiotemporal data, demonstrating the effectiveness of introducing the nonlinear fitting ability of neural networks in modelling spatial non-stationarity. ~~Additionally, statistical analyses confirm the presence of significant spatial heterogeneity in~~

It is noteworthy that, as a deep learning model, GNNWR does require more time than traditional models to fit the given dataset. For the above experiment on PM2.5 ~~concentrations, which the model effectively elucidates~~ dataset, it takes 2000 epochs for GNNWR to optimize the network's parameters and minimize the loss, which is about 3 minutes in a CPU (Intel Core i5-12400) environment. Nevertheless, compared to the advantages in model performance, such a time-consumption is acceptable, especially considering that a CUDA-enabled GPU can further accelerate the process.

Owing to the intimate association between model analysis and spatial aspects, the GNNWR furnishes a range of spatial visualization functionalities grounded in the folium. By instantiating the `Visualize` object, we can render
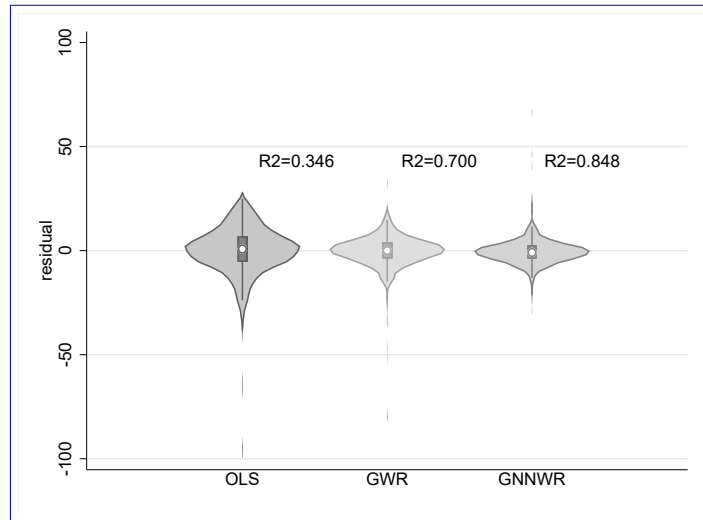
Figure 4. The residual distributions and R^2 indicator for OLS, GWR and GNNWR on PM2.5 dataset.

various model variables within a spatial context. The `Visualize` object proffers multiple visualization techniques, encompassing the visualization of internal datasets within the model, heatmaps of coefficients, and the visualization of spatial points. Figure 5 illustrates the spatial distribution of the dependent variable PM2.5 across the dataset. Notably, PM2.5 concentrations are elevated in the North China and Xinjiang regions, in contrast to the relatively lower levels observed in Yunnan and the northern reaches of Inner Mongolia.

```
>>> import gnnwr.utils as utils
>>> visualizer = utils.Visualize(data=gnnwr,lon_lat_columns=['lng','lat'])
>>> visualizer.display_dataset(name='all',y_column='PM2_5')
```

The `coefs_heatmap` function facilitates the visual representation of the spatial distribution of independent variable coefficients, thereby enriching our comprehension of the impact of individual independent variables on the dependent variable across varying geographical contexts. Figure 6 depicts the distinctive spatial distribution patterns of AOD coefficients.

```
>>> visualizer.coefs_heatmap('coef_aod_sat')
```

Through these visualization techniques, we can perceptively comprehend the analysis outcomes of the model. They offer abundant functionality that enables us to better understand the spatial behavior of the model and gain a more profound insight into the model's performance and spatial relationships.

Concurrently, the visualization output of the Visualize object is in HTML format, permitting researchers to manipulate the map via zooming, panning, and rotation. During the manipulation of the map, the visualization of the data will alter according to the scale of the map. When the map scale is small, the points in the spatial
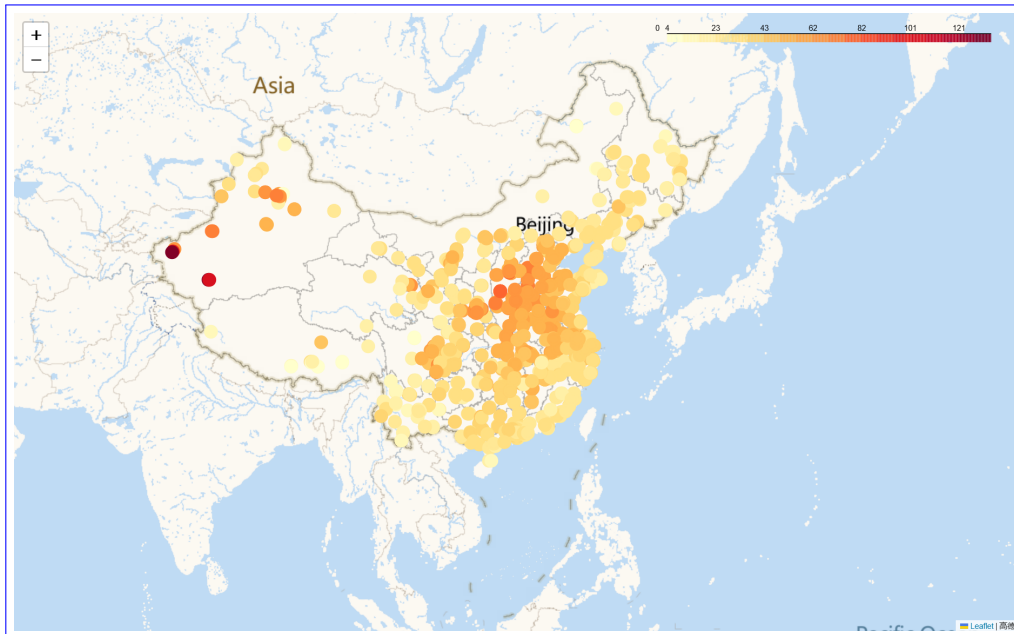
Figure 5. ~~Schematic diagram~~ Diagram of the spatial distribution of PM2.5. Redder points represent higher PM2.5 values.

Figure 6. ~~Schematic diagram~~ Diagram of AOD coefficient distribution. Darker areas highlight regions with strong positive correlations, indicating high levels of particulate matter.

distribution are dense, necessitating the clustering and display of these points to preserve clarity. Conversely, when the map scale is large, the information of the points at specific locations will be displayed. This facilitates detailed inspection and analysis of geographic data to cater to diverse research requirements.

3.2.4 Saving and reusing

Upon the successful completion of training a model, the frequent need arises to reuse said model. To facilitate this process, the model repository incorporates a dedicated `load_model` function, which is specifically purposed to reload model files that were automatically saved during the training progression. Notably, the repository ~~retains~~ maintains only the neural network-related components, specifically the neural network architecture and parameters, within the model. Consequently, when reusing a model, the recommended sequence is as follows: initially, construct an instance correspondent to the model's architectural design, before subsequently calling the `load_model` method to import the parameters and weights.

3.2.5 Prediction

Ultimately, we can employ the prediction method to forecast other datasets. Prior to generating predictions, it is essential to transform the other datasets into the `predictDataset` class, which is integrated within the GNNWR package. This transformation can be accomplished by utilizing the `init_predict_dataset` method. This method computes the distance vectors between the features in the dataset to be predicted and the reference points, and applies the identical scaling transformation to the independent variables as in the training dataset, guaranteeing ~~the reliability of the prediction outcomes~~ that the input for the model inference follows the same statistical distribution of the training data. The prediction method yields a Pandas' DataFrame comprising the original data and the predicted results. Moreover, when employing the GNNWR model for analysis, spatial weights are of paramount importance. These weights signify the spatial variability of the influence of each independent variable on the dependent variable. To acquire spatial weights, the `predict_weight` method can be utilized to output the pertinent information. Figure 7 presents a geographical visualization of the GNNWR model's predictive outcomes.

```
>>> from gnnwr.datasets import init_predict_dataset
>>> pred_dataset = init_predict_dataset(data = pred_data,
...                                     train_dataset = train_set,
...                                     x_column=x_column,
...                                     spatial_column=spatial_column)
>>> res = gnnwr.predict(pred_dataset)
```
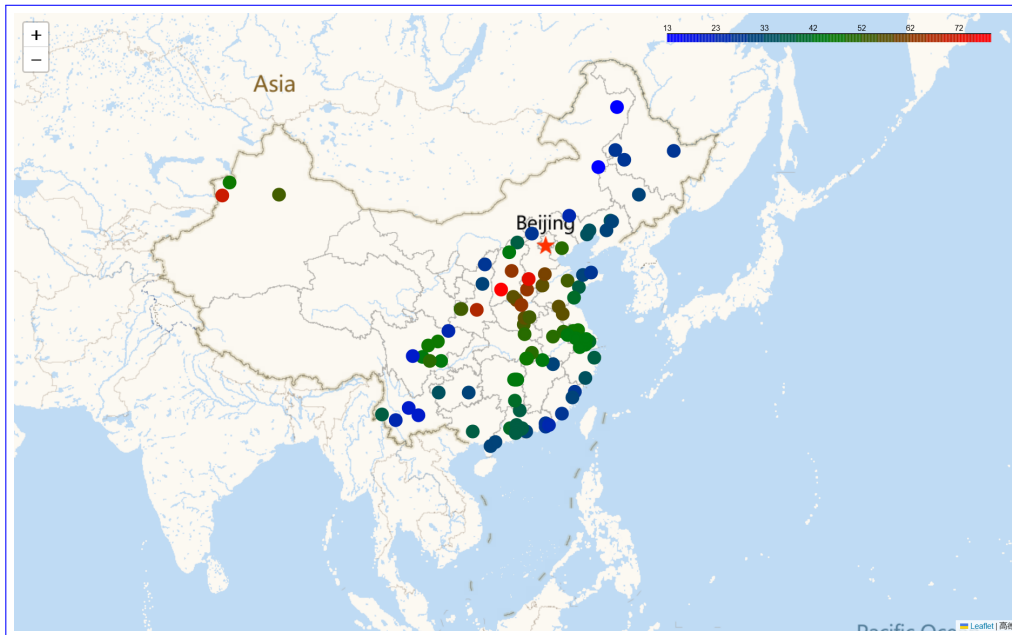
Figure 7. Geospatial Visualization of GNNWR Model Predictions for PM2.5. Red points indicate higher PM2.5 predictions; blue points indicate lower PM2.5 predictions.

3.3 Usage Example for GTNNWR

The workflow of employing GTNNWR is largely akin to that of the GNNWR model. We exemplify this by utilizing daily surface dissolved silicate (DSi) concentration data from the offshore waters of Zhejiang. This study utilized the GTNNWR approach to retrieve the distribution of coastal DSi concentrations, addressing the challenges posed by spatiotemporal non-stationarity (Qi et al., 2023).

3.3.1 Dataset initialization

Similar to the GNNWR model, data preprocessing is essential when utilizing the GTNNWR model to acquire a data format that the model can process as well. The GTNNWR model is specifically tailored for spatiotemporal data, wherein the regression coefficients perpetually vary in both space and time. Consequently, the data processed by the model must possess spatiotemporal attributes. When employing the `init_dataset`~~function~~ function, designating the time data as the time dimension can generate valid input for the GTNNWR model. This function computes the time distance vectors based on the distance calculation method specified by the `temporal_fun` parameter and subsequently employs them as input features for each sampling point. The default time distance calculation method is the Manhattan distance.

```
>>> train_set, val_set, test_set = init_dataset(data=data,
```

```
...                                          test_ratio=0.15,
...                                          valid_ratio=0.1,
445 ...                                       x_column=x_column,
...                                          y_column=y_column,
...                                          spatial_column=spatial_column,
...                                          temp_column=temp_column)
```

3.3.2 Model configuration and running

450 `GTNNWR` is designed as a subclass incorporated within the the GNNWR package, inheriting from its foundational `GNNWR` class. As a result, it retains the same set of methods inherent to its superclass. The instantiation process for the GTNNWR model closely mirrors that of GNNWR, with the primary difference lying in the input format for hidden layers—a two-element two-dimensional list. This unique input configuration stems from GTNNWR's integration strategy, which involves employing a STPNN to compute spatiotemporal proximities and then feeding
455 these computations into a STWNN for determining spatiotemporal weights. Specifically, the first list in this input designates the hidden layer structure of STPNN, whereas the second list delineates the hidden layer architecture pertaining to STWNN.

~~The GNNWR package features a novel learning rate adjustment mechanism that is employed by default in conjunction with the SGD optimizer. The seminal paper on GTNNWR consistently utilizes this adjustment technique~~
460 ~~throughout model training (Wu et al., 2021). The process commences with the minimum learning rate, progressively scaling in a stepwise fashion to the maximum learning rate, and then sustaining this peak rate for a designated duration. Thereafter, the learning rate undergoes exponential decay until it reaches a predetermined threshold, beyond which it is maintained at a lower fixed value . The adjustment mechanism's hyperparameters encompass the minimum and maximum learning rates, the decay rate, as well as the number of epochs dedicated to the growth,~~
465 ~~stabilization, and the decay phase.~~

The procedure for training an instantiated model with data, as well as the tasks of printing model metadata and exhibiting the outcomes of training, aligns with the methodologies employed in the previous exemplar.

```
    1: >>> gtnnwr = models.GTNNWR(train_set, val_set, test_set)
470 2: >>> gtnnwr.run(max_epoch = 5000,early_stop=200,print_frequency = 200)
    3: >>> optimizer_params = {
    4: ...        "maxlr": 0.025,
    5: ...        "minlr": 0.010,
    6: ...        "upepoch": 1000,
475 7: ...        "decayepoch": 2000,
    8: ...        "decayrate": 0.998,
    9: ...        "stop_change_epoch": 5000,
```

```
10: ...        "stop_lr": 0.01,
11: ... }
12: >>> Layers = [[3], [1024, 512, 256,128,64,32]]
13: >>> gtnnwr = models.GTNNWR(train_set, val_set, test_set,
14: ...                     Layers,
15: ...                     optimizer='SGD',
16: ...                     optimizer_params=optimizer_params,
17: ...                     # drop_out=0.3,
18: ...                     model_name="GTNNWR_DSi",
19: ...                     model_save_path="./demo_result/gtnnwr_models",
20: ...                     log_path="./demo_result/gtnnwr_logs/",
21: ...                     write_path="./tf-logs/gtnnwr_runs")
22: >>> gtnnwr.run(max_epoch = 4000)
23: >>> gtnnwr.result()
```

```
1: -------------------Model Information----------------
2: Model Name:          | GTNNWR_DSi
3: independent variable: | ['refl_b01', 'refl_b02', 'refl_b03',
4:                         'refl_b04', 'refl_b05', 'refl_b07']
5: independent variable: | ['refl_b01', 'refl_b02', 'refl_b03', 'refl_b04', 'refl_b05', 'refl_b07']
6: dependent variable:   | ['SiO3']
7: %DIF >
8: OLS coefficients:
9: x0: 6.84114
10: x1: 1.63606
11: x2: 0.11273
12: x3: -5.76276
13: x4: 1.62136
14: x5: -2.69205
15: Intercept: 1.05858
16: %DIF >
17: -------------------Result Information---------------
18: Test Loss: |                0.16295
19: Test R2   : |                0.69155
20: Train R2  : |                0.75372
```

```
21: Valid R2 : |                          0.81317
22: RMSE: |                               0.40367
23: AIC:  |                              453.26982
24: AICc: |                              453.26016
25: F1:   |                                0.19419
26: F2:   |                               -8.26737
27: f3_param_0: |                         27.48529
28: f3_param_1: |                          0.12909
29: f3_param_2: |                          0.95790
30: f3_param_3: |                          2.41443
31: f3_param_4: |                         18.00247
32: f3_param_5: |                         28.71637
33: f3_param_6: |                        271.65698
34: Test Loss: |                           0.16574
35: Test R2  : |                           0.68628
36: Train R2 : |                           0.71628
37: Valid R2 : |                           0.75261
38: RMSE: |                                0.40711
39: AIC:  |                              460.66438
40: AICc: |                              463.34515
41: F1:   |                                0.22449
42: F2:   |                              -12.20421
43: f3_param_0: |                         27.02276
44: f3_param_1: |                          0.12710
45: f3_param_2: |                          0.94117
46: f3_param_3: |                          2.37350
47: f3_param_4: |                         17.69786
48: f3_param_5: |                         28.23304
49: f3_param_6: |                        267.06781
```

According to various model indicators, utilizing neural networks to estimate the spatiotemporal non-stationarity of DSi is indeed effective. The model successfully achieved an R^2 value of 0.692 on the test set, values of 0.716, 0.752 and 0.686 on the training, validation and testing set, respectively, effectively reconstructing the distribution of silicate in the offshore waters of Zhejiang. As indicated by Figure 8, such coefficients of determination are much higher than those of traditional models like OLS and GTWR (implemented with the `mgtwr` package by Sun, version 2.0.5); also,

the residuals of GTNNWR are generally smaller than OLS and GTWR. These outstanding performances demonstrate
550 GTNNWR's superior performance in capturing the spatiotemporal non-stationarity of DSi concentrations.
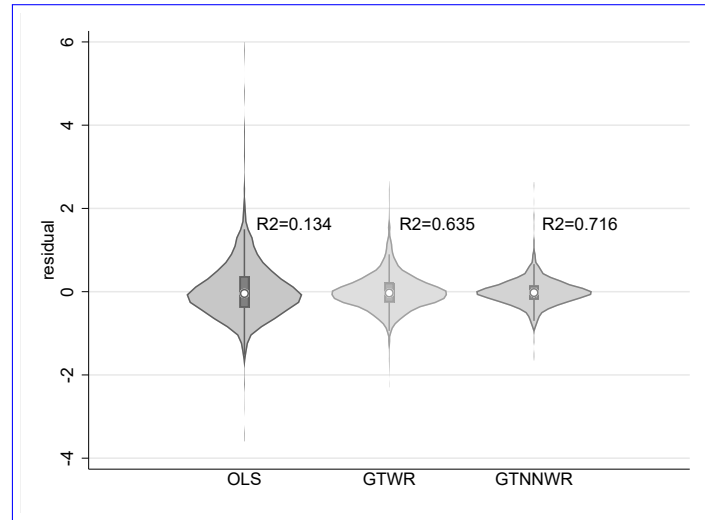
Figure 8. The residual distributions and R^2 indicator for OLS, GTWR and GTNNWR on DSi dataset.

3.3.3 Result and visualization

In order to investigate the variability of coefficients for distinct variables across different samples, one can leverage
the `reg_result` function to achieve this goal. The function computes and systematically arranges each sample's
coefficient values into a Pandas' `DataFrame` format, thereby outputting the results. With the resultant coefficient
555 matrix in hand, researchers can then conduct targeted analyses pertinent to specific spatial processes. For instance,
we can visualize the coefficients of each variable by employing time and space as three-dimensional coordinate axes
(Figure 9). This enables us to directly observe the relationship between the bands of remote sensing images and
silicate concentrations at different spatial locations. By integrating relevant prior knowledge, we can interpret the
outcomes of the model.

4 Conclusions

560

This study introduces the GNNWR package, a Python-based model repository designed to facilitate spatiotemporal
intelligent regression modeling. The package is constructed on PyTorch, a widely employed deep learning frame-
work, and affords a comprehensive workflow for simulating geographical processes characterized by spatiotemporal
non-stationarity. The GNNWR package optimizes intricate procedures encompassing data preprocessing, network
565 architecture formulation, model training, and result computation, thereby enhancing user accessibility. It enables in-
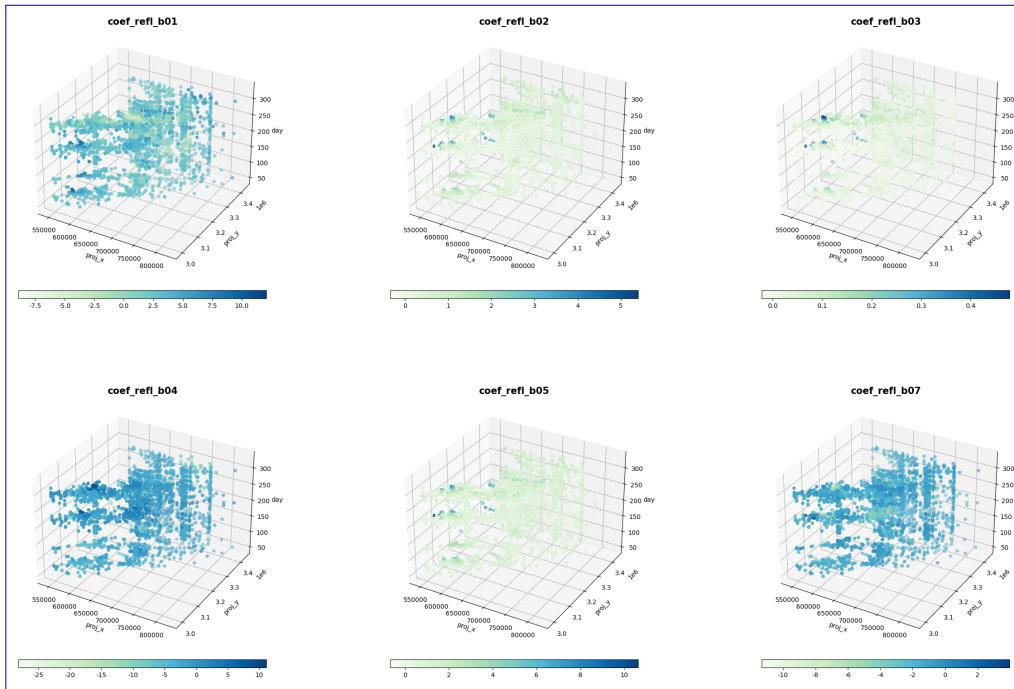
Figure 9. ~~Visualization results of model~~ Model coefficients in a 3D space-time coordinate system. Blue dots represent a greater positive effect of the variable on silicate concentration; lighter dots represent a smaller effect.

dividuals with limited programming expertise to quickly master the application of pertinent models such as GNNWR and GTNNWR for the estimation of spatiotemporal non-stationary processes.

~~The GNNWR model family exhibits substantial promise in addressing spatiotemporal non-stationarity, effectively capturing complex nonlinear relationships inherent in the interplay between spatiotemporal proximity and non-stationary weights. Employing advanced neural network techniques, these models enhance the precision of discerning spatiotemporal non-stationary features. Additionally, the exploration of spatiotemporal non-stationarity facilitates an in-depth examination of spatial analytical patterns and the underlying mechanisms governing geographical processes. The GNNWR and GTNNWR models empower researchers to derive more accurate and reliable insights across diverse domains within the context of geographical information~~ The integrated visualization functionalities further augment the package's utility, allowing users to interpret model outcomes and their spatial relationships more effectively.

However, the GNNWR package is not without limitations. The GNNWR and GTNNWR models are computationally intensive, particularly for large datasets. Also, training neural networks requires substantial computational resources, which may limit accessibility for some users. Future works should focus on optimizing the computational efficiency, implementing parallel processing techniques and optimizing the model architecture are potential methods that can significantly reduce computation times. Data handling is another area that can be improved, incorporating techniques

for spatiotemporal data augmentation and pre-processing can make the models more robust and applicable to a wider range of datasets.

~~The~~ Besides, the scholarly understanding of spatiotemporal non-stationarity is progressing, driving the continual evolution of GNNWR-based models and the emergence of diverse derivatives, such as geographically convolutional neural network weighted regression ~~(?)~~ (Dai et al., 2022) and directional geographically weighted neural network Regression ~~(?)~~ (Wu et al., 2019). These model variants have substantially augmented the functionalities of GNNWR across various dimensions. Moving forward, we are committed to enhancing the model library by leveraging the current framework and integrating a variety of network and data architectures to create novel extension models. This expansion will enhance the package's capability to incorporate a wide range of modeling techniques for addressing spatiotemporal non-stationarity. Consequently, this broadening of capabilities will extend the applicability of the models, encompassing a more comprehensive array of spatiotemporal analytical approaches.

Code and data availability. The GNNWR package version used in this article is 0.1.11, which can be found at https://pypi. python.org/pypi/gnnwr. The project's hosting and development are both ongoing on https://github.com/zjuwss/gnnwr (Yin et al., 2024a)(https://doi.org/10.5281/zenodo.10890176), and the relevant documents can be found at https://gnnwr.github. io.All the examples mentioned in this article, supported by research papers, can be retrieved from Yin et al. (2024b)(https://doi.org/10.5281/zenodo.13270526). We strongly encourage readers to replicate, adapt, and undertake additional experiments using this open-source package.

Author contributions. YZY, DJL, LY, QJ, and WSS initially developed the package and spearheaded its subsequent evolution. Notably, substantial code enhancements were made by YZY, DJL, LY, WRX, WYG, QJ, CYJ, WSS, and DZH. Each author actively participated in the design discourse and offered critical feedback on the evolving codebase. The manuscript was primarily composed by YZY, WRX, and WYG, with substantive input from all co-authors.

Competing interests. The authors declare that they have no conflict of interest.

Acknowledgements. This work was supported by the National Natural Science Foundation of China ~~(grant 42271466~~[No. 42225605, 42001323, 423B1001~~)~~], National Key Research and Development Program of China ~~(grant~~ [No. 2021YFB3900902~~)~~], Provincial Key R&D Program of Zhejiang ~~(grant~~ [No. 2021C01031~~)~~], Fundamental Research Funds for the Central Universities ~~(grant~~ [No. 2022FZZX01-05~~)~~]. This work was also supported by the Deep-time Digital Earth (DDE) Big Science Program and the Earth System Big Data Platform of the School of Earth Sciences, Zhejiang University.

References

Ahadnejad Reveshty, M., Heydari, M. T., and Tahmasebimoghaddam, H.: Spatial Analysis of the Factors Impacting on the Spread of Covid-19 in the Neighborhoods of Zanjan, Iran, Spatial Information Research, https://doi.org/10.1007/s41324-023-00550-0, 2023.

Bivand, R. and Yu, D.: spgwr: Geographically Weighted Regression, https://cran.r-project.org/package=spgwr, 2023.

Brunsdon, C., Fotheringham, A. S., and Charlton, M. E.: Geographically Weighted Regression: A Method for Exploring Spatial Nonstationarity, Geographical Analysis, 28, 281–298, https://doi.org/https://doi.org/10.1111/j.1538-4632.1996.tb00936.x, 1996.

Brunsdon, C., Fotheringham, A. S., and Charlton, M.: Some Notes on Parametric Significance Tests for Geographically Weighted Regression, Journal of Regional Science, 39, 497–524, https://doi.org/https://doi.org/10.1111/0022-4146.00146, 1999.

Chen, Y., Wu, S., Wang, Y., Zhang, F., Liu, R., and Du, Z.: Satellite-Based Mapping of High-Resolution Ground-Level PM2.5 with VIIRS IP AOD in China through Spatially Neural Network Weighted Regression, Remote Sensing, 13, https://doi.org/10.3390/rs13101979, 2021.

Dai, Z., Wu, S., Wang, Y., Zhou, H., Zhang, F., Huang, B., and Du, Z.: Geographically Convolutional Neural Network Weighted Regression: A Method for Modeling Spatially Non-Stationary Relationships Based on a Global Spatial Proximity Grid, International Journal of Geographical Information Science, 36, 2248–2269, https://doi.org/10.1080/13658816.2022.2100892, 2022.

Du, Z.: GNNWR Code and Simulated Data, https://doi.org/10.6084/m9.figshare.11375826, 2019.

Du, Z., Wang, Z., Wu, S., Zhang, F., and Liu, R.: Geographically neural network weighted regression for the accurate estimation of spatial non-stationarity, International Journal of Geographical Information Science, 34, 1–25, https://doi.org/10.1080/13658816.2019.1707834, 2020a.

Du, Z., Wu, S., Wang, Z., Wang, Y., Zhang, F., and Liu, R.: Estimating Ground-Level PM2.5 Concentrations Across China Using Geographically Neural Network Weighted Regression, Journal of Geo-information Science, 22, 122, https://doi.org/10.12082/dqxxkx.2020.190533, 2020b.

Du, Z., Qi, J., Wu, S., Zhang, F., and Liu, R.: A Spatially Weighted Neural Network Based Water Quality Assessment Method for Large-Scale Coastal Areas, Environmental Science & Technology, 55, 2553–2563, https://doi.org/10.1021/acs.est.0c05928, 2021.

Fotheringham, A. S., Crespo, R., and Yao, J.: Geographical and Temporal Weighted Regression (GTWR), Geographical Analysis, 47, 431–452, https://doi.org/https://doi.org/10.1111/gean.12071, 2015.

Fotheringham, A. S., Yang, W., and Kang, W.: Multiscale Geographically Weighted Regression (MGWR), Annals of the American Association of Geographers, 107, 1247–1265, https://doi.org/10.1080/24694452.2017.1352480, 2017.

Georganos, S. and Kalogirou, S.: A Forest of Forests: A Spatially Weighted and Computationally Efficient Formulation of Geographical Random Forests, ISPRS International Journal of Geo-Information, 11, https://doi.org/10.3390/ijgi11090471, 2022.

Guo, B., Wang, X., Pei, L., Su, Y., Zhang, D., and Wang, Y.: Identifying the Spatiotemporal Dynamic of PM2.5 Concentrations at Multiple Scales Using Geographically and Temporally Weighted Regression Model Across China During 2015-2018, Science of The Total Environment, 751, https://doi.org/10.1016/j.scitotenv.2020.141765, 2021.

Hagenauer, J. and Helbich, M.: A Geographically Weighted Artificial Neural Network, International Journal of Geographical Information Science, 36, 215–235, https://doi.org/10.1080/13658816.2021.1871618, 2022.

Han, L., Zhou, W., and Li, W.: Fine Particulate PM 2.5 Dynamics During Rapid Urbanization in Beijing, 1973–2013, Scientific Reports, 6, srep23 604, https://doi.org/10.1038/srep23604, 2016.

He, J., Wei, Y., and Yu, B.: Geographically Weighted Regression Based on a Network Weight Matrix: A Case Study Using Urbanization Driving Force Data in China, International Journal of Geographical Information Science, 37, 1209–1235, https://doi.org/10.1080/13658816.2023.2192122, 2023.

He, Q. and Huang, B.: Satellite-Based Mapping of Daily High-Resolution Ground PM2.5 in China via Space-Time Regression Modeling, Remote Sensing of Environment, 206, 72–83, https://doi.org/10.1016/j.rse.2017.12.018, 2018.

Huang, B., Wu, B., and Barry, M.: Geographically and Temporally Weighted Regression for Modeling Spatio-Temporal Variation in House Prices, International Journal of Geographical Information Science, 24, 383–401, https://doi.org/10.1080/13658810802672469, 2010.

Leung, Y., Mei, C.-L., and Zhang, W.-X.: Statistical Tests for Spatial Nonstationarity Based on the Geographically Weighted Regression Model, Environment and Planning A: Economy and Space, 32, 9–32, https://doi.org/10.1068/a3162, 2000.

Lewandowska-Gwarda, K.: Geographically Weighted Regression in the Analysis of Unemployment in Poland, ISPRS International Journal of Geo-Information, 7, https://doi.org/10.3390/ijgi7010017, 2018.

Liang, M., Zhang, L., Wu, S., Zhu, Y., Dai, Z., Wang, Y., Qi, J., Chen, Y., and Du, Z.: A High-Resolution Land Surface Temperature Downscaling Method Based on Geographically Weighted Neural Network Regression, Remote Sensing, 15, https://doi.org/10.3390/rs15071740, 2023.

Liu, C., Wu, S., Dai, Z., Wang, Y., Du, Z., Liu, X., and Qiu, C.: High-Resolution Daily Spatiotemporal Distribution and Evaluation of Ground-Level Nitrogen Dioxide Concentration in the Beijing–Tianjin–Hebei Region Based on TROPOMI Data, Remote Sensing, 15, https://doi.org/10.3390/rs15153878, 2023.

Lu, B., Charlton, M., Harris, P., and Fotheringham, A. S.: Geographically Weighted Regression with a Non-Euclidean Distance Metric: A Case Study Using Hedonic House Price Data, International Journal of Geographical Information Science, 28, 660–681, https://doi.org/10.1080/13658816.2013.865739, 2014.

Lu, B., Harris, P., Charlton, M., Brunsdon, C., Nakaya, T., Murakami, D., Gollini, I., Hu, Y., and Evans, F. H.: GWmodel: Geographically-Weighted Models, http://gwr.nuim.ie/, 2024.

Ma, X., Zhang, J., Ding, C., and Wang, Y.: A Geographically and Temporally Weighted Regression Model to Explore the Spatiotemporal Influence of Built Environment on Transit Ridership, Computers, Environment and Urban Systems, 70, 113–124, https://doi.org/10.1016/j.compenvurbsys.2018.03.001, 2018.

McKinney, W. et al.: Data Structures for Statistical Computing in Python, Austin, TX, 2010.

Ni, S., Wang, Z., Wang, Y., Wang, M., Li, S., and Wang, N.: Spatial and Attribute Neural Network Weighted Regression for the Accurate Estimation of Spatial Non-Stationarity, ISPRS International Journal of Geo-Information, 11, 620, https://doi.org/10.3390/ijgi11120620, 2022.

680 Oshan, T. M., Li, Z., Kang, W., Wolf, L. J., and Fotheringham, A. S.: mgwr: A Python Implementation of Multiscale Geographically Weighted Regression for Investigating Process Spatial Heterogeneity and Scale, https://pypi.org/project/mgwr/, accessed from the ISPRS International Journal of Geo-Information, 2019.

Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., Killeen, T., Lin, Z., Gimelshein, N., Antiga, L., Desmaison, A., Kopf, A., Yang, E., DeVito, Z., Raison, M., Tejani, A., Chilamkurthy, S., Steiner, B., Fang, L., Bai,
685 J., and Chintala, S.: PyTorch: An Imperative Style, High-Performance Deep Learning Library, in: Advances in Neural Information Processing Systems, vol. 32, Curran Associates, Inc., https://papers.nips.cc/paper_files/paper/2019/hash/bdbca288fee7f92f2bfa9f7012727740-Abstract.html, 2019.

Qi, J., Du, Z., Wu, S., Chen, Y., and Wang, Y.: A Spatiotemporally Weighted Intelligent Method for Exploring Fine-Scale Distributions of Surface Dissolved Silicate in Coastal Seas, Science of The Total Environment, 886, 163 981,
690 https://doi.org/10.1016/j.scitotenv.2023.163981, 2023.

Shen, Y., de Hoogh, K., Schmitz, O., Clinton, N., Tuxen-Bettman, K., Brandt, J., Christensen, J. H., Frohn, L. M., Geels, C., Karssenberg, D., Vermeulen, R., and Hoek, G.: Europe-Wide Air Pollution Modeling from 2000 to 2019 Using Geographically Weighted Regression, Environment International, 178, https://doi.org/10.1016/j.envint.2023.108111, 2023.

Sisman, S. and Aydinoglu, A. C.: A Modelling Approach with Geographically Weighted Regression Methods for Deter-
695 mining Geographic Variation and Influencing Factors in Housing Price: A Case in Istanbul, Land Use Policy, 119, https://doi.org/10.1016/j.landusepol.2022.106183, 2022.

Stein, R. E., Conley, J. F., and Davis, C.: The Differential Impact of Physical Disorder and Collective Efficacy: A Geographically Weighted Regression on Violent Crime, GeoJournal, 81, 351–365, https://doi.org/10.1007/s10708-015-9626-6, 2015.

700 Sun, K.: mgtwr, https://pypi.org/project/mgtwr, 2024.

Team, R. C.: R: A Language and Environment for Statistical Computing, R Foundation for Statistical Computing, Vienna, Austria, https://www.R-project.org/, 2017.

van Rossum, G.: Python Programming Language, https://www.python.org/, 2011.

Wang, Y., Niu, Y., Li, M., Yu, Q., and Chen, W.: Spatial Structure and Carbon Emission of Urban Agglomerations: Spatiotem-
705 poral Characteristics and Driving Forces, Sustainable Cities and Society, 78, https://doi.org/10.1016/j.scs.2021.103600, 2022.

Wheeler, D.: Fits Geographically Weighted Regression Models with Diagnostic Tools, https://cran.r-project.org/package=gwrr, 2022.

Wu, J., Xia, L., Chan, T., Awange, J., and Zhong, B.: Downscaling Land Surface Temperature: A Framework Based on
710 Geographically and Temporally Neural Network Weighted Autoregressive Model with Spatio-Temporal Fused Scaling Factors, ISPRS Journal of Photogrammetry and Remote Sensing, pp. 259–272, https://doi.org/10.1016/j.isprsjprs.2022.03.009, 2022.

Wu, S.: Simulated datasets and codes of GTNNWR, https://doi.org/10.6084/m9.figshare.12355472.v1, 2020.

Wu, S., Du, Z., Wang, Y., Lin, T., and Liu, R.: Modeling Spatially Anisotropic Nonstationary Processes in Coastal Envi-
715 ronments Based on a Directional Geographically Neural Network Weighted Regression, Science of The Total Environment, 709, 136 097, https://doi.org/10.1016/j.scitotenv.2019.136097, 2019.

Wu, S., Wang, Z., Du, Z., Huang, B., Zhang, F., and Liu, R.: Geographically and Temporally Neural Network Weighted Regression for Modeling Spatiotemporal Non-stationary Relationships, International Journal of Geographical Information Science, 35, 582–608, https://doi.org/10.1080/13658816.2020.1775836, 2021.

720   Yang, Q., Yuan, Q., Yue, L., Li, T., Shen, H., and Zhang, L.: The Relationships Between PM2.5 and Aerosol Optical Depth (AOD) in Mainland China: About and Behind the Spatio-Temporal Variations, Environmental Pollution, 248, 526–535, https://doi.org/10.1016/j.envpol.2019.02.071, 2019.

Yang, Y., Wang, H., Qin, S., Li, X., Zhu, Y., and Wang, Y.: Analysis of Urban Vitality in Nanjing Based on a Plot Boundary-Based Neural Network Weighted Regression Model, ISPRS International Journal of Geo-Information, 11, 624, https://doi.org/10.3390/ijgi11120624, 2022.

725   Yin, Z., Ding, J., Liu, Y., Wang, R., Wang, Y., Qi, J., Chen, Y., Wu, S., and Du, Z.: GNNWR v0.1.11: A Python package for modeling spatial temporal non-stationary, https://doi.org/10.5281/zenodo.10890176, 2024a.

Yin, Z., Ding, J., Liu, Y., Wang, R., Wang, Y., Qi, J., Chen, Y., Wu, S., and Du, Z.: Replication package for GNNWR v0.1.11: A Python package for modeling spatial temporal non- stationary, https://doi.org/10.5281/zenodo.13270526, 2024b.