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

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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 (GNNWR) and Geographically and Temporally Neural Network Weighted Regression (GTNNWR), which using neural networks to estimate the spatiotemporal non-stationarity. Due to the higher accuracy and generalization ability, these models have been widely used in various fields of scientific research. To facilitate the 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.,

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 functions (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 software package `mgwr` that focuses on multi-scale estimation and efficient computation of spatial non-stationarity (Oshan et al., 2019). It supplements the R-language-based open-source tools, e.g., `spgwr` (Bivand and Yu, 2023), `gwrr` (Wheeler, 2022), and `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 geographical 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 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 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 (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 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 (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).

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 (STPNN) to accurately generate space-time distance and extended GNNWR with the STPNN to incorporate temporal effects into 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 et al., 2023), environmental modeling (Wu et al., 2019; Du et al., 2021; Wu et al., 2022; Qi et al., 2023) and urban geography (Wang et al., 2022; Yang et al., 2022; Liang et al., 2023). 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, 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 in different fields, and to solicit feedbacks for refinement and enhancement of these models.

This research has developed an open-source Python package, denoted as the `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 visualizations. 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 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 package. 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 Ordinary Least squares Regression (OLR) model is expressed as:

$$y_i = \beta_0^{OLR} + \sum_{k=1}^{p} \beta_k^{OLR} x_{ik} + \varepsilon_i \quad \text{for } i = 1, 2, \ldots, n \tag{1}$$

where y_i and x_{ik} are the dependent variable 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.

Considering the spatial non-stationarity, the GWR model extends OLR approach to enable spatially localized estimates, by allowing local variations in rates of change. Thus, regression can be represented as:

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

where $\beta_0(u_i, v_i)$ 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:

$$\hat{\boldsymbol{\beta}}(u_i, v_i) = (\mathbf{X}^\top \mathbf{W}(u_i,\ v_i)\mathbf{X})^{-\mathbf{1}} \mathbf{X}^\top \mathbf{W}(u_i, v_i)\mathbf{y} \tag{3}$$

where $\mathbf{W}(u_i, v_i)$ 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:

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

where d_{ij} is the distance between fit point i and its neighbor j.

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 is calculated as follows:

$$\boldsymbol{W}(u_i, v_i) = \mathrm{SWNN}([d_{i1}^S, d_{i2}^S, \ldots, d_{in}^S]^\top) \tag{5}$$

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

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

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

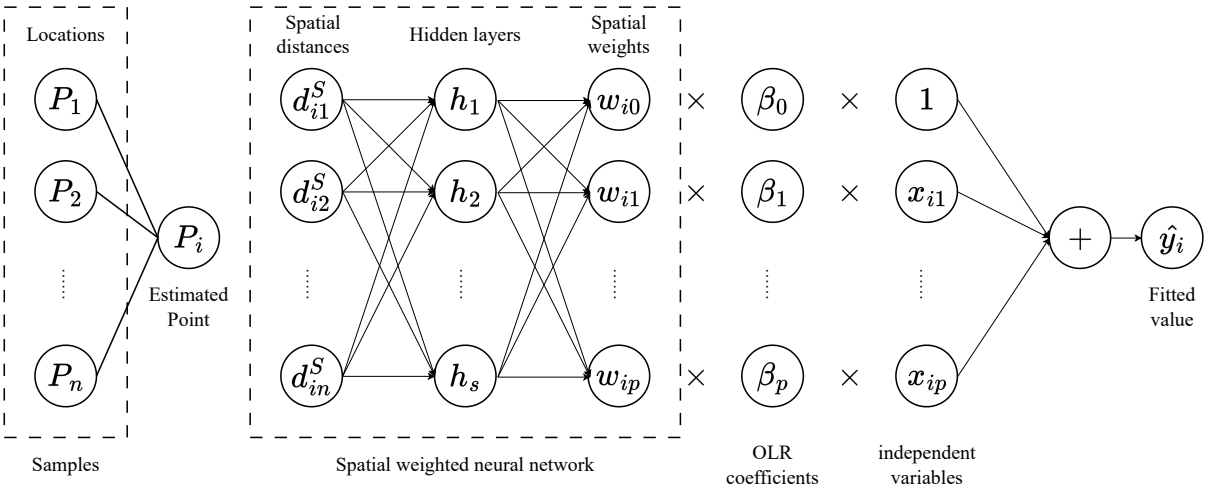

Figure 1. The framework of the GNNWR model.

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 form:

$$\begin{aligned} y_i &= \beta_0(u_i, v_i, t_i) + \sum_{k=1}^{p} \beta_k(u_i, v_i, t_i) x_{ik} + \varepsilon_i, \quad \text{for } i = 1, 2, \ldots, n \\ &= w_0(u_i, v_i, t_i)\beta_0^{OLR} + \sum_{k=1}^{p} w_k(u_i, v_i, t_i)\beta_k^{OLR} x_{ik} + \varepsilon_i, \quad \text{for } i = 1, 2, \ldots, n \end{aligned} \tag{8}$$

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 designed a spatiotemporal weighted neural network (STWNN) calculate the spatiotemporal weights as follows:

$$\boldsymbol{W}(u_i, v_i, t_i) = \mathrm{STWNN}\left(\left[d_{i1}^{ST}, d_{i2}^{ST}, \ldots, d_{in}^{ST}\right]^{\top}\right) \tag{9}$$

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:

$$d_{ij}^{ST} = d_{ij}^{S} \otimes d_{ij}^{T} \tag{10}$$

where 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 the spatiotemporal dimension, Wu et al. (2021) proposed 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 (Figure 2):

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

The spatiotemporal weights are then integrated with global OLR estimates, generating continuous space-time 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 $\boldsymbol{S}$ is the hat matrix of the GTNNWR model.

3 Package Descriptions

In this section, we present a comprehensive overview of the `gnnwr` package (version 0.1.11) and the range of models it supports. We begin by introducing the fundamental architecture of the software package, 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.

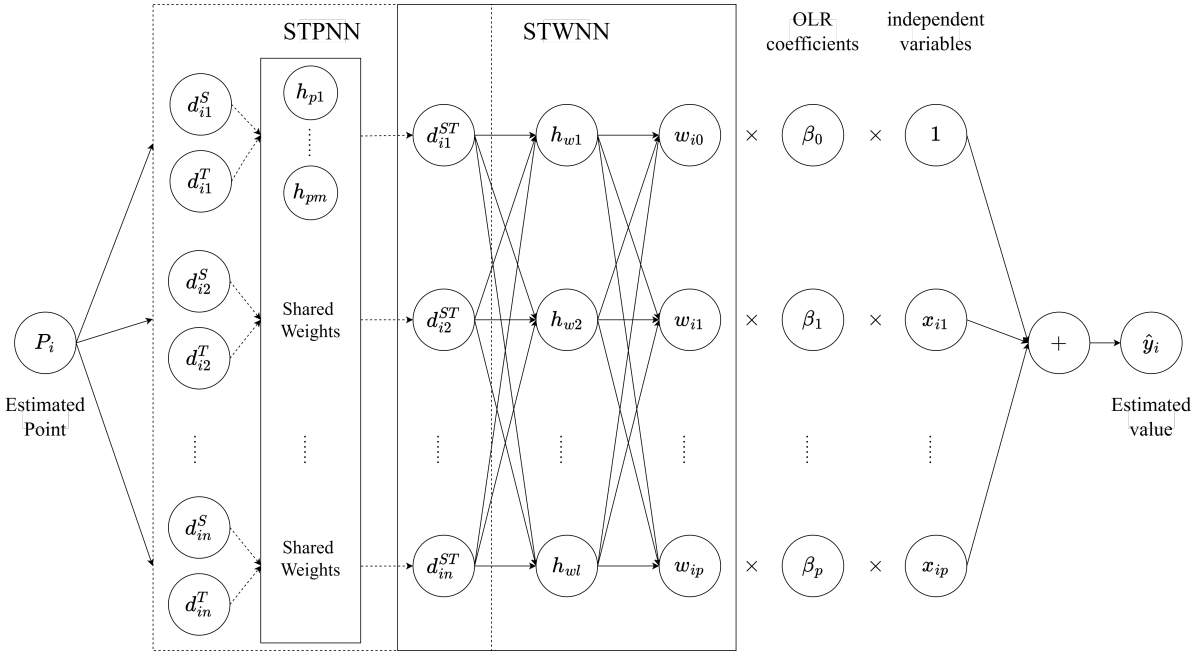

Figure 2. The framework of the GTNNWR model. d_{ij}^S and d_{ij}^T represent the spatial distance and temporal distance between the estimated points P_i and P_j, respectively. The spatiotemporal proximity d_{ij}^{ST} is obtained by integrating d_{ij}^S and d_{ij}^T through the STPNN.

3.1 Package Architecture

The `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` 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.

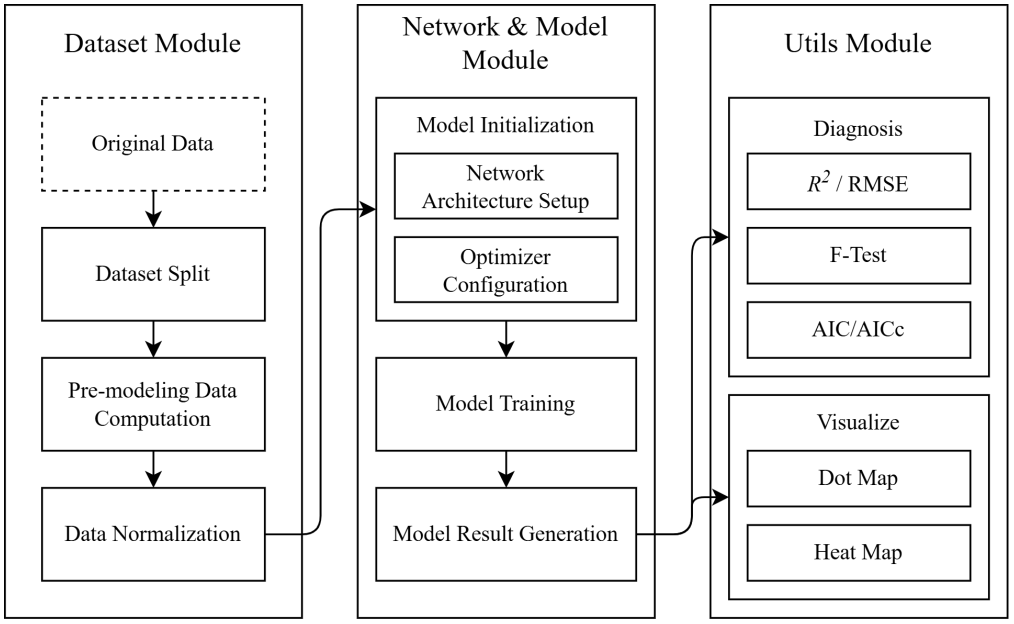

Figure 3. Workflow diagram of the package. Dashed boxes denote the raw data, solid boxes represent the code process modules, and arrows indicate the direction of data flow.

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 randomly divides the dataset into training, validation 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.

```
>>> from gnnwr.datasets import init_dataset
>>> train_set, val_set, test_set = init_dataset(data=data,
...                                             test_ratio=0.15,
...                                             valid_ratio=0.1,
...                                             x_column=x_column,
...                                             y_column=y_column,
...                                             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 Parametric Rectified Linear Unit (PReLU) function with an initial value of 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 0.6, 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.

```
>>> from gnnwr import models
>>> from torch import nn
>>> gnnwr = models.GNNWR(train_dataset = train_set,
...                      valid_dataset = val_set,
...                      test_dataset = test_set,
...                      dense_layers = [1024, 512, 256, 128],
...                      activate_func = nn.PReLU(init=0.2),
...                      start_lr = 0.6,
...                      optimizer = "Adadelta",
...                      drop_out = 0.2,
...                      batch_norm = True,
...                      model_name = "GNNWR_PM25")
```

```
>>> 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()

--------------------Model Information-----------------
Model Name:           | GNNWR_PM25
independent variable: | ['dem', 'w10', 'd10', 't2m', 'aod_sat', 'tp']
dependent variable:   | ['PM2_5']

OLS coefficients:
x0: 7.12861
x1: -4.03670
x2: -1.90988
x3: 21.29951
x4: 36.57638
x5: -24.50677
Intercept: 19.16957
```

```
--------------------Result Information----------------
Test Loss: |                  33.42091
Test R2  : |                   0.84280
Train R2 : |                   0.84762
Valid R2 : |                   0.84541
RMSE: |                        5.78108
AIC:  |                     1257.37056
AICc: |                     1254.68787
F1:   |                        0.11974
F2:   |                        3.52673
f3_param_0: |                  1.81630
f3_param_1: |                 19.05118
f3_param_2: |                  0.42682
f3_param_3: |                 68.13538
f3_param_4: |                 47.61187
f3_param_5: |                170.05663
f3_param_6: |                122.83797
```

The empirical results reveal that the model exhibits robust performance in the reconstruction of PM2.5 distributions, 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 0.848 for the training dataset, 0.845 for the validation dataset, and 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.

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 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 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

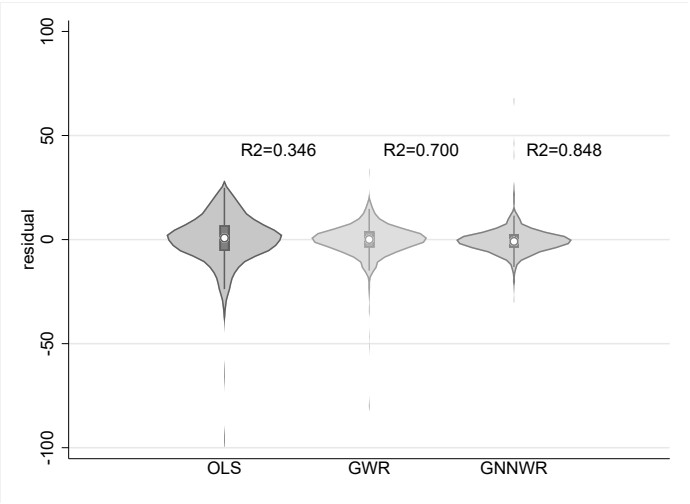

Figure 4. The residual distributions and R^2 indicator for OLS, GWR and GNNWR on PM2.5 dataset.

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 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.

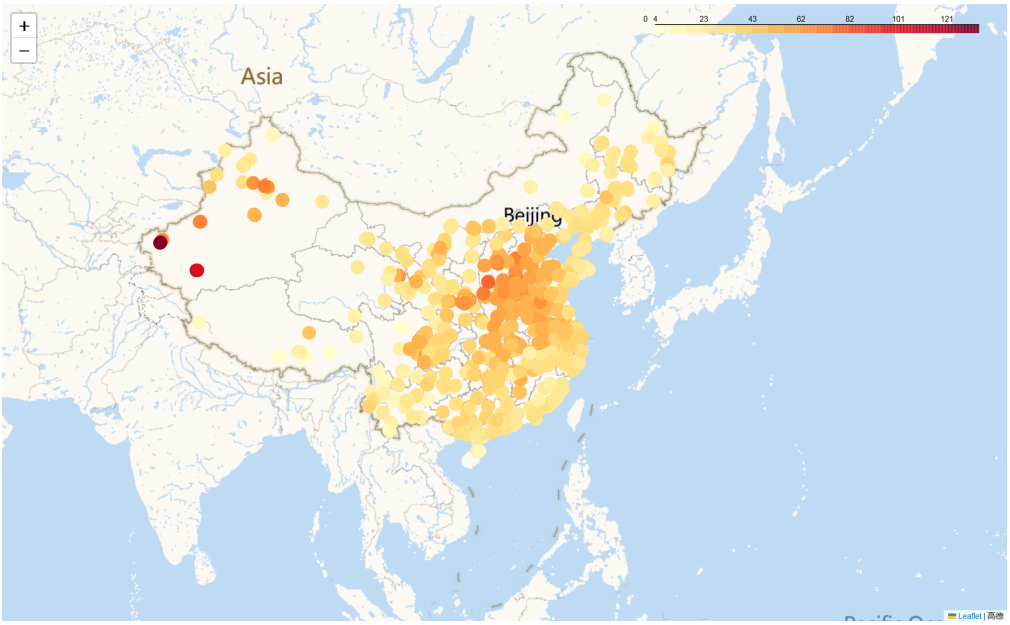

Figure 5. Diagram of the spatial distribution of PM2.5. Redder points represent higher PM2.5 values. Map crafted using Python's folium library with Gaode basemap.

Figure 6. Diagram of AOD coefficient distribution. Darker areas highlight regions with strong positive correlations, indicating high levels of particulate matter. Map crafted using Python's folium library with Gaode basemap.

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 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 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)
```

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).

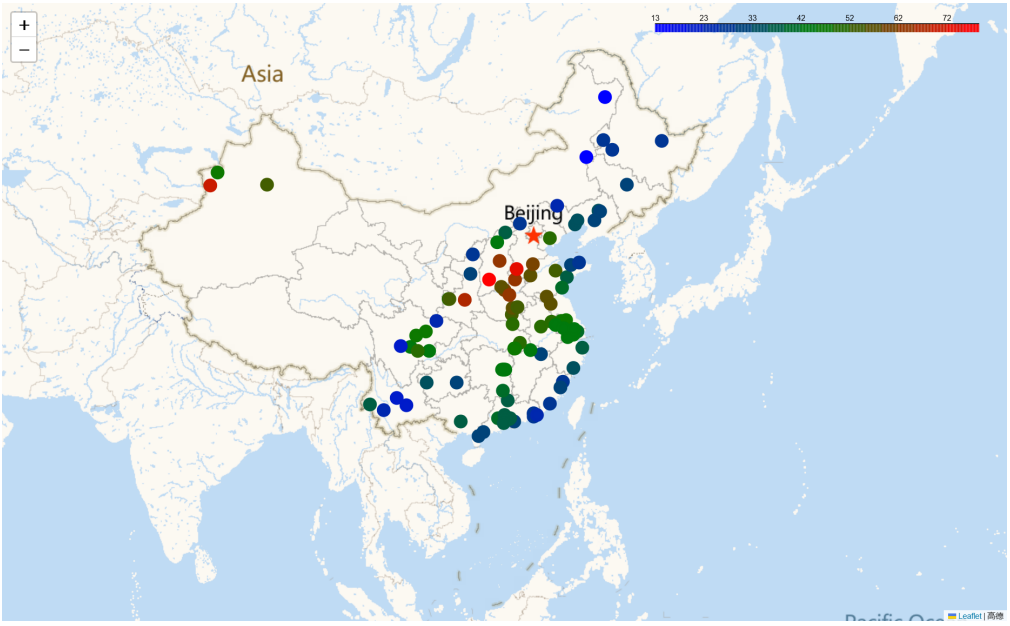

Figure 7. Geospatial Visualization of GNNWR Model Predictions for PM2.5. Red points indicate higher PM2.5 predictions; blue points indicate lower PM2.5 predictions. Map crafted using Python's folium library with Gaode basemap.

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, 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,
...                                             x_column=x_column,
...                                             y_column=y_column,
...                                             spatial_column=spatial_column,
...                                             temp_column=temp_column)
```

3.3.2 Model configuration and running

`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 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 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.

```
>>> optimizer_params = {
...     "maxlr": 0.025,
...     "minlr": 0.010,
...     "upepoch": 1000,
...     "decayepoch": 2000,
...     "decayrate": 0.998,
...     "stop_change_epoch": 5000,
...     "stop_lr": 0.01,
... }
>>> Layers = [[3], [1024, 512, 256,128,64,32]]
>>> gtnnwr = models.GTNNWR(train_set, val_set, test_set,
...                        Layers,
...                        optimizer='SGD',
...                        optimizer_params=optimizer_params,
...                        # drop_out=0.3,
...                        model_name="GTNNWR_DSi",
...                        model_save_path="./demo_result/gtnnwr_models",
...                        log_path="./demo_result/gtnnwr_logs/",
...                        write_path="./tf-logs/gtnnwr_runs")
>>> gtnnwr.run(max_epoch = 4000)
>>> gtnnwr.result()

--------------------Model Information-----------------
Model Name:           | GTNNWR_DSi
```

```
independent variable: | ['refl_b01', 'refl_b02', 'refl_b03', 'refl_b04', 'refl_b05', 'refl_b07']
dependent variable:   | ['SiO3']

OLS coefficients:
x0: 6.84114
x1: 1.63606
x2: 0.11273
x3: -5.76276
x4: 1.62136
x5: -2.69205
Intercept: 1.05858

--------------------Result Information----------------
Test Loss: |                    0.16574
Test R2  : |                    0.68628
Train R2 : |                    0.71628
Valid R2 : |                    0.75261
RMSE: |                        0.40711
AIC:  |                      460.66438
AICc: |                      463.34515
F1:   |                        0.22449
F2:   |                      -12.20421
f3_param_0: |                 27.02276
f3_param_1: |                  0.12710
f3_param_2: |                  0.94117
f3_param_3: |                  2.37350
f3_param_4: |                 17.69786
f3_param_5: |                 28.23304
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 R^2 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 GTNNWR's superior performance in capturing the spatiotemporal non-stationarity of DSi concentrations.

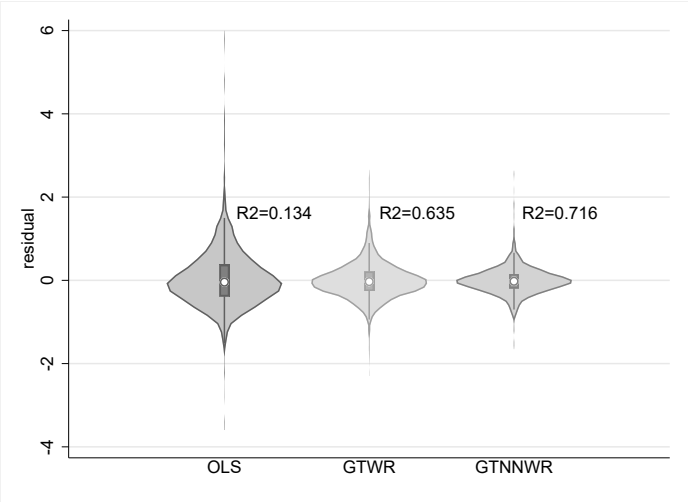

Figure 8. The residual distributions and R^2 indicator for OLS, GTWR and GTNNWR on DSi dataset.

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 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

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 framework, and affords a comprehensive workflow for simulating geographical processes characterized by spatiotemporal non-stationarity. The GNNWR package optimizes intricate procedures encompassing data preprocessing, network architecture formulation, model training, and result computation, thereby enhancing user accessibility. It enables individuals with limited programming expertise to quickly master the application of pertinent models such as GN-

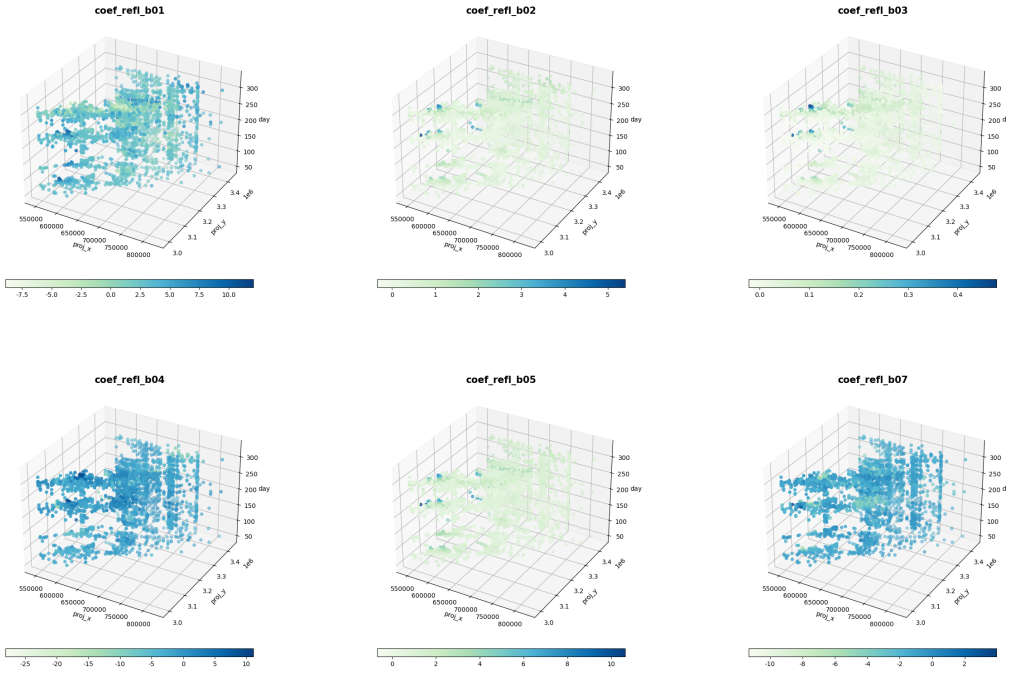

Figure 9. Model coefficients in a 3D space-time coordinate system. Blue dots represent a greater positive effect of the variable on silicate concentration; lighter dots represent a smaller effect.

NWR and GTNNWR for the estimation of spatiotemporal non-stationary processes. 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.

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, DJL, WRX, and WYG, with substantive input from all co-authors.

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

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