

# **Geospatial Artificial Intelligence**

## **AI In Geography And Urban Science**

**May 28<sup>th</sup>, 2024**

## □ Three Stages Of Method Application

- Learning New Methods And Constructing A Comprehensive Framework;
- Adapting Methods to New Research Scenarios;
- Optimizing Methods Based on Research Insights.

## □ Principles Of Selecting Examples

- **Topic:** Human Behaviors;
- **Characteristic Of Data:** Short-term High-frequency Fluctuations.

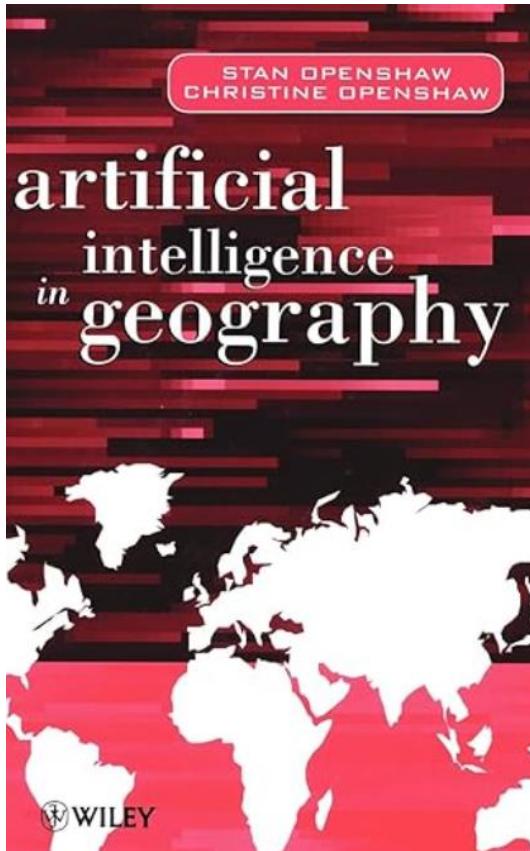
## Several Vital Questions For Comprehending GeoAI:

- **Why** AI is needed for traditional topics in geography and urban science?
- **What** specific questions can be better addressed through the integration of GeoAI?
  - **How** is GeoAI applied to the aforementioned research scenarios?
- **What** new challenges have arisen with the application of GeoAI?
  - **How** does GeoAI contribute to solving the identified questions?
- **What** new applications might GeoAI have in the future?

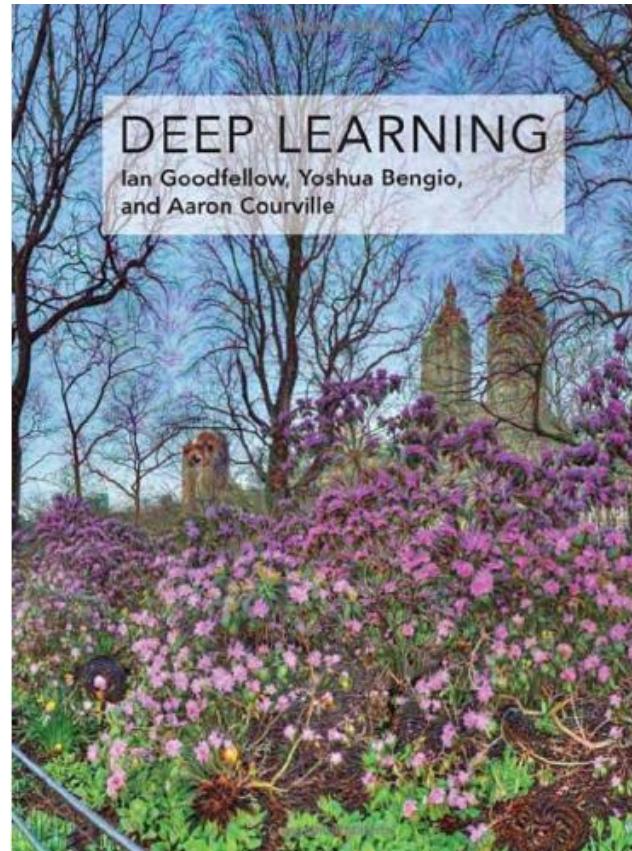
# Outline

- Basic Topics In Urban Science and Geography
- Conception And Case Studies Of GeoAI
- Applications Of GeoAI In Urban Science
- Problems And Challenges Of GeoAI

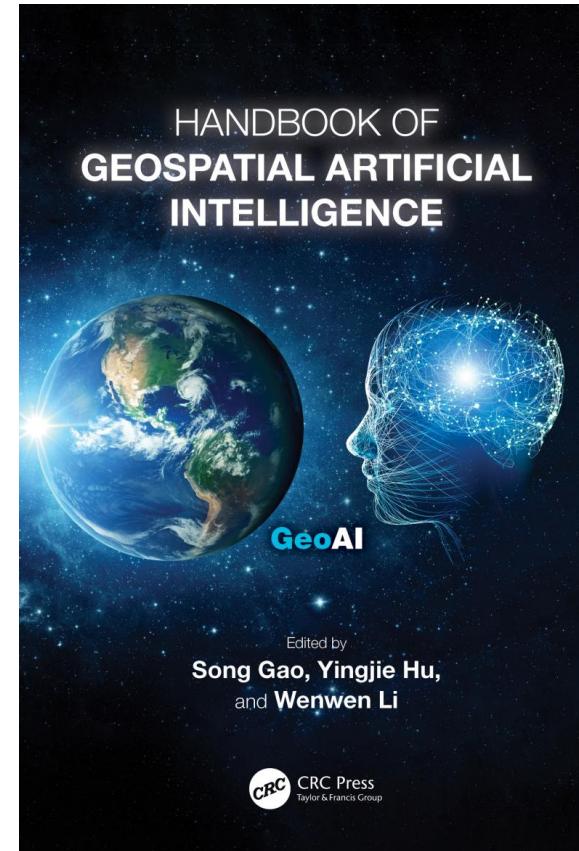
# Recommended Reading List



S. Openshaw & C. Openshaw, 1997



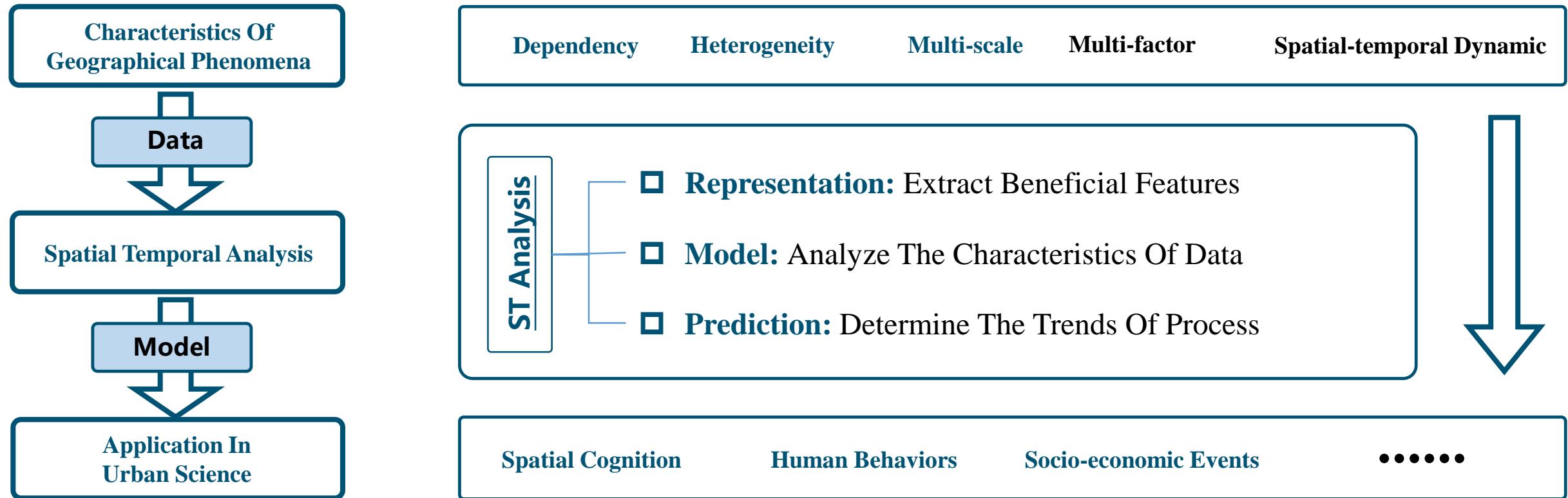
<https://www.deeplearningbook.org/>  
Goodfellow et al, 2016



Gao et al, 2023

# Main Theme

- Develop spatial-temporal data statistical analysis and mining methods tailored for **complex and dynamic** geographic processes.



# **Basic Topics In Urban Science and Geography**

# Spatiality Of Geographic Phenomena

- Classical statistical theories assume **independent samples**, which limits their ability to comprehend the **spatiality of geographic phenomena**.



## □ Spatial Dependence

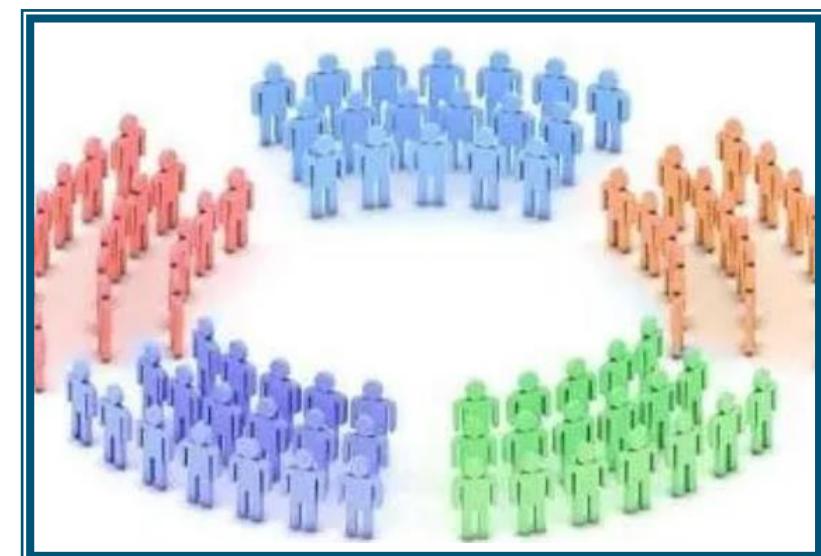
Everything is related to everything else, but near things are more related than distant things.

— Waldo R . Tobler, 1970

## □ Spatial Heterogeneity

Geographic variables exhibit uncontrolled variance.

— Michael F . Goodchild, 2004



Birds of a feather flock together

# Spatiality Of Geographic Phenomena

- Based on the spatiality of geographic phenomena, researchers need to recognize both the similarities and disparities among **phenomena/behaviors** in terms of **space** and **place**.



- The study of geographic distributions over the Earth's surface. The study of local differences in phenomena over the Earth' s surface was the keynote

—A. Hettner, 1927



- To provide accurate, orderly, and rational **description** and **interpretation** of the variable character of the earth surface.

—R. Hartshorne, 1959



Here is a simple case: **Simpson's Paradox**

	Boy		Girl	
	Applicants	Admission	Applicants	Admission
Total	8442	44%	4321	35%

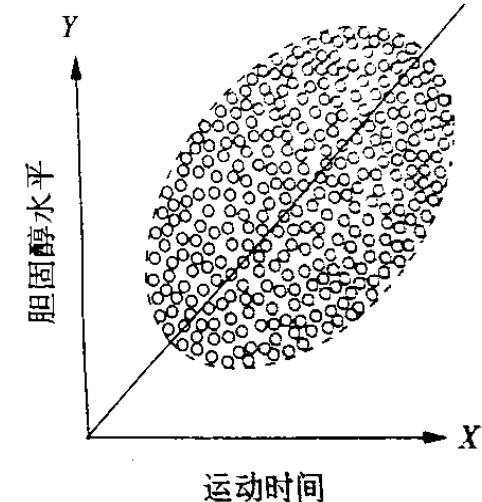
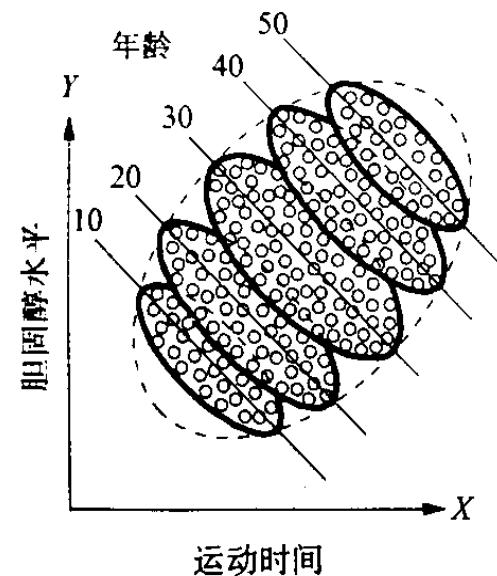
Is there gender discrimination  
based on the admission rate of this school?

	Boy		Girl	
College	Applicants	Admission	Applicants	Admission
A	825	62%	108	82%
B	560	63%	25	68%
C	325	37%	593	34%
D	417	33%	375	35%
E	191	28%	393	24%
F	373	6%	341	7%

Is there gender discrimination based on the admission rate of the  
school's colleges?

## Simpson's Paradox In The Diagram

Simpson 's paradox is a phenomenon in probability and statistics in which a trend appears in several groups of data but disappears or reverses when the groups are combined. This result is particularly problematic when frequency data are unduly given causal interpretations.



Urban science and geographical research focus on space, but there is **no natural spatial analysis unit**, which may lead to the following issues.:

- Modifiable Areal Unit Problem(MAUP)
- Ecological Fallacy

## MAUP: With changes in scale and zones, both spatial autocorrelation and spatial heterogeneity undergo variations.



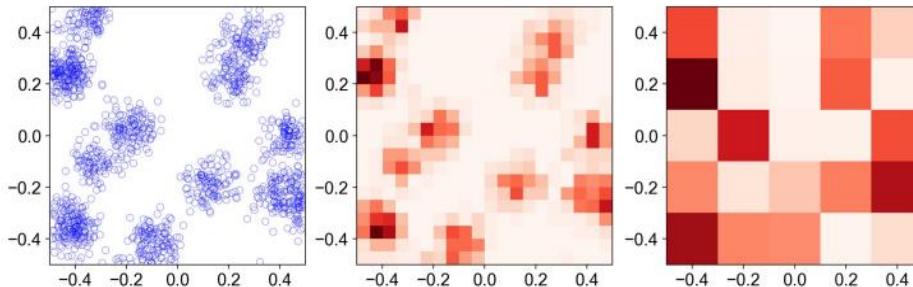
Environment and Planning A, 1984, volume 16, pages 17–31

### Ecological fallacies and the analysis of areal census data

S Openshaw

Department of Geography, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, England  
Received 7 June 1982; in revised form 23 December 1982

**Abstract.** In many countries census data are only reported for areal units and not at the individual level. This custom raises the spectre of ecological fallacy problems. In this paper, a 10% sample census (from the United Kingdom) and individual census data (from Italy) are used to provide an empirical demonstration of the nature and magnitude of these problems. It is concluded that ecological fallacy effects are endemic to areal census data, although their magnitude is perhaps not as large as might have been expected. The principal difficulty is that there is at present no way of predicting in advance the degree of severity likely to be associated with particular variables and particular techniques. Finally, a suggestion is made concerning how the potentially serious practical consequences can be reduced.



21 Régions (RE)



22 Large squares (LS)



341 Employment Areas (EA)



341 Small squares (SS)

scale effect (size)  
zoning effect (shape)

# Representation

## Representation: What types of data?

- Field, Network, Relational Model...
- Spatially Intensive Data, Spatially Extensive Data...
  - **Spatially Intensive Data:** When spatial aggregation occurs, quantities such as temperature and elevation should not be cumulated. It often used in tasks such as trend surface analysis and surface modeling;
  - **Spatially Extensive Data:** When spatial aggregation occurs, quantities such as human activities can be accumulated. It has irregular sampling, rich attributes, and is often used in tasks such as correlation analysis and regression prediction.

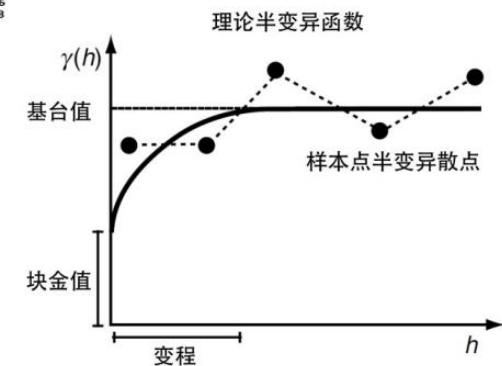
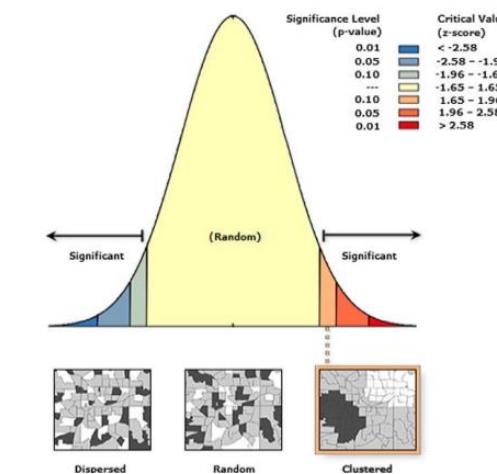
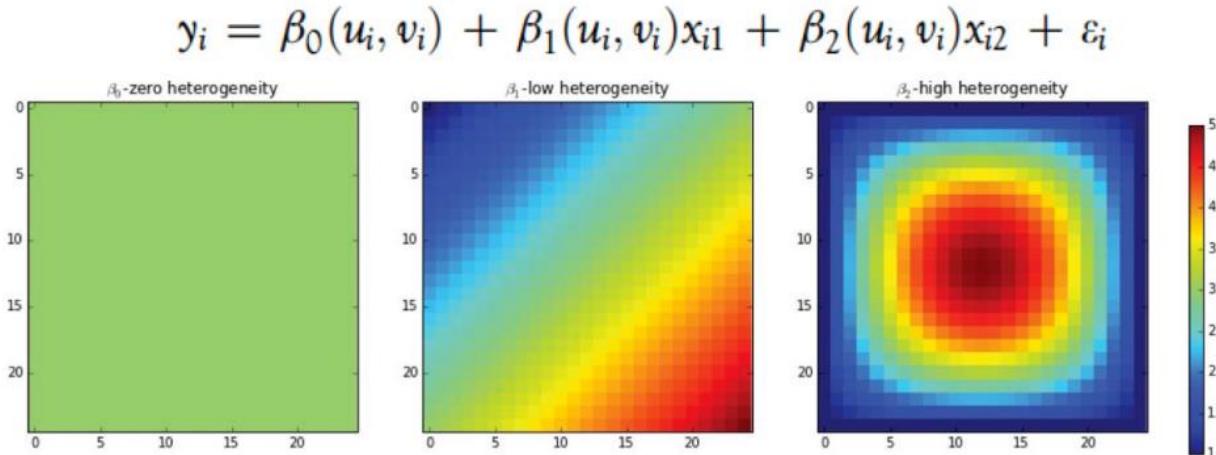


## How to explore the patterns of geospatial data?

### □ What characteristics should be considered? □ Which methods are commonly used?

- Spatial Autocorrelation;
- Spatial Heterogeneity;
- Geographic Similarity…

- Spatial Statistics;
- Geostatistics…



Tobler, W. R. (1970). A Computer Movie Simulating Urban Growth in the Detroit Region. *Economic Geography*, 46, 234–240.

Goodchild, M. F. (2004). The validity and usefulness of laws in geographic information science and geography. *Annals of the Association of American Geographers*, 94(2), 300-303.

Zhu, A. X., Lu, G., Liu, J., Qin, C. Z., & Zhou, C. (2018). Spatial prediction based on Third Law of Geography. *Annals of GIS*, 24(4), 225-240.

## How to model spatiality?

### □ Spatial Weights Matrix

- Representation of data structure.

### □ Construction Methods

- Binary Weighting;
- Variable Weighting…



$$W = \begin{bmatrix} w_{11} & w_{12} & \dots & w_{1n} \\ w_{21} & w_{22} & \dots & w_{2n} \\ \dots & \dots & \dots & \dots \\ w_{n1} & w_{n2} & \dots & w_{nn} \end{bmatrix}$$

Spatial Weights Matrix

### □ Example 1

**Moran's autocorrelation coefficient** is an extension of **Pearson product-moment correlation coefficient** to a univariate series.

$$\square \text{ Pearson Correlation Coefficient } \rho = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}}$$

$$\square \text{ Moran' I: } I = \frac{n \sum_i \sum_{i \neq j} w_{ij} (y_i - \bar{Y})(y_j - \bar{Y})}{(\sum_i \sum_{i \neq j} w_{ij}) \sum_i (y_i - \bar{Y})^2}$$

### □ Example 2: Model the influence of podium

- The influence of the podium is not only affected by **the lecturer** but also related to **the attributes of other areas** in the classroom.

□ Assumption of homogeneous influence:  $Y_i = \sum_{i \neq j} \beta Y_j + \mu_i$

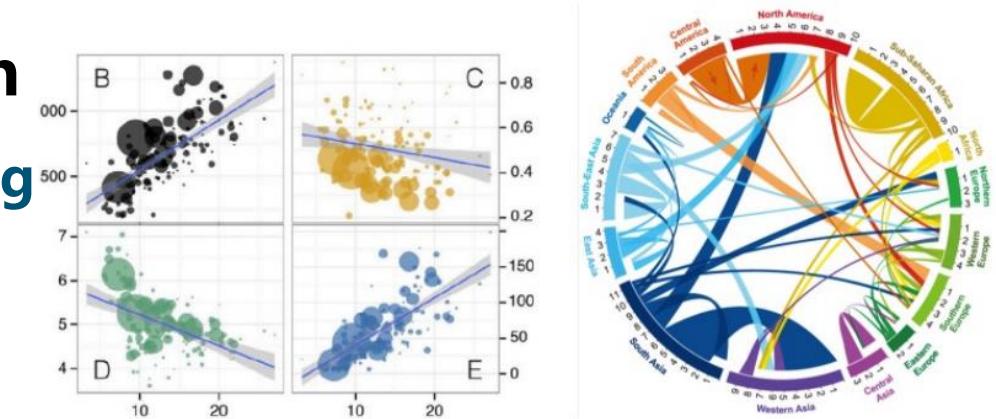
□ Assumption of heterogeneous influence:  $Y_i = \sum_{i \neq j} W_{ij} Y_j + \mu_i$

# Prediction

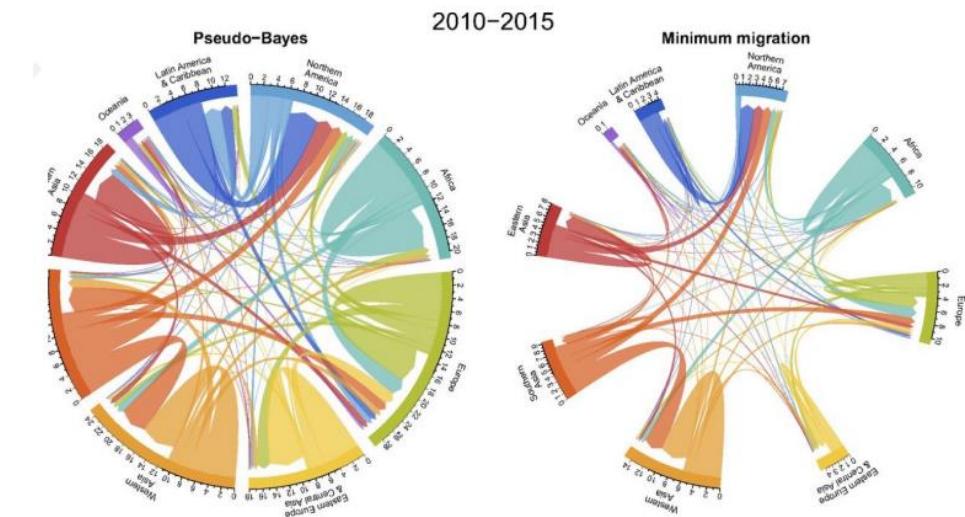
## The necessity of spatio-temporal prediction

### □ Data incompleteness under spatiotemporal slicing

- Sparse and incomplete spatial distribution;
- Spatial interactions that difficult to observe;
- Misalignment of Measurement:
  - Scale、Sample、Geographical Context etc.



Distribution of Intercontinental  
Immigration Flow →

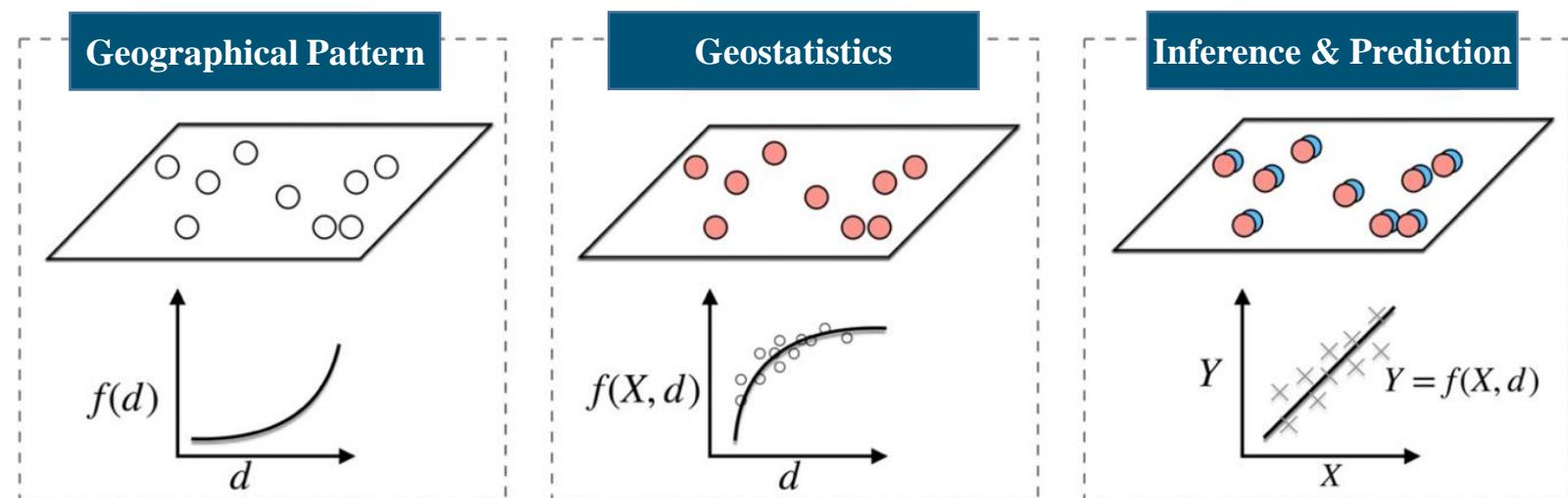


Abel, G. J., & Sander, N. (2014). Quantifying global international migration flows. *Science*, 343(6178), 1520-1522.

Azose, J. J., & Raftery, A. E. (2019). Estimation of emigration, return migration, and transit migration between all pairs of countries. *Proceedings of the National Academy of Sciences*, 116(1), 116-122.

## Develop advancing methods to represent, model, and predict geospatial phenomena with non-stationary spatiotemporal dynamics.

- Traditional GIS modeling approaches fail to enable algorithms to understand **diverse geographic phenomena**.
- The classical statistical and spatial econometric methods based on **the assumption of spatial stationarity** cannot model **complex spatial mechanisms**;
- The incomplete spatiotemporal information restricts researchers' ability to accurately predict the **developmental trends** of geographic phenomena.



# **Conception And Case Studies Of GeoAI**

## □ Conception And Case Studies Of GeoAI

- Introduction to Machine Learning(ML) and Artificial Intelligence(AI)
- The Conceptualization Of GeoAI
- The Relationship Between Geospatial Phenomena And AI
  - Representation Of Geographical Phenomena
  - Model Of Geographical Phenomena
  - Prediction Of Geographical Trend
- Several New Issues Faced by GeoAI

## AI, ML And DL

- Artificial Intelligence(AI)
- Machine Learning(ML)
- Deep Learning(DL)

AI, ML And DL  
The Relationship Among the Three Conception→

### Artificial Intelligence

Programs that perceive their environment  
and take actions to achieving defined goals.

### Machine Learning

Algorithms that can learn from data  
and generalize to unseen data and thus  
perform tasks without instructions.

### Deep Learning

Deep learning is the subset  
of machine learning  
methods based on neural  
network with representation  
learning.

# Task Of Machine Learning

## Classification

- How can a program reliably differentiate between a fork and a car?

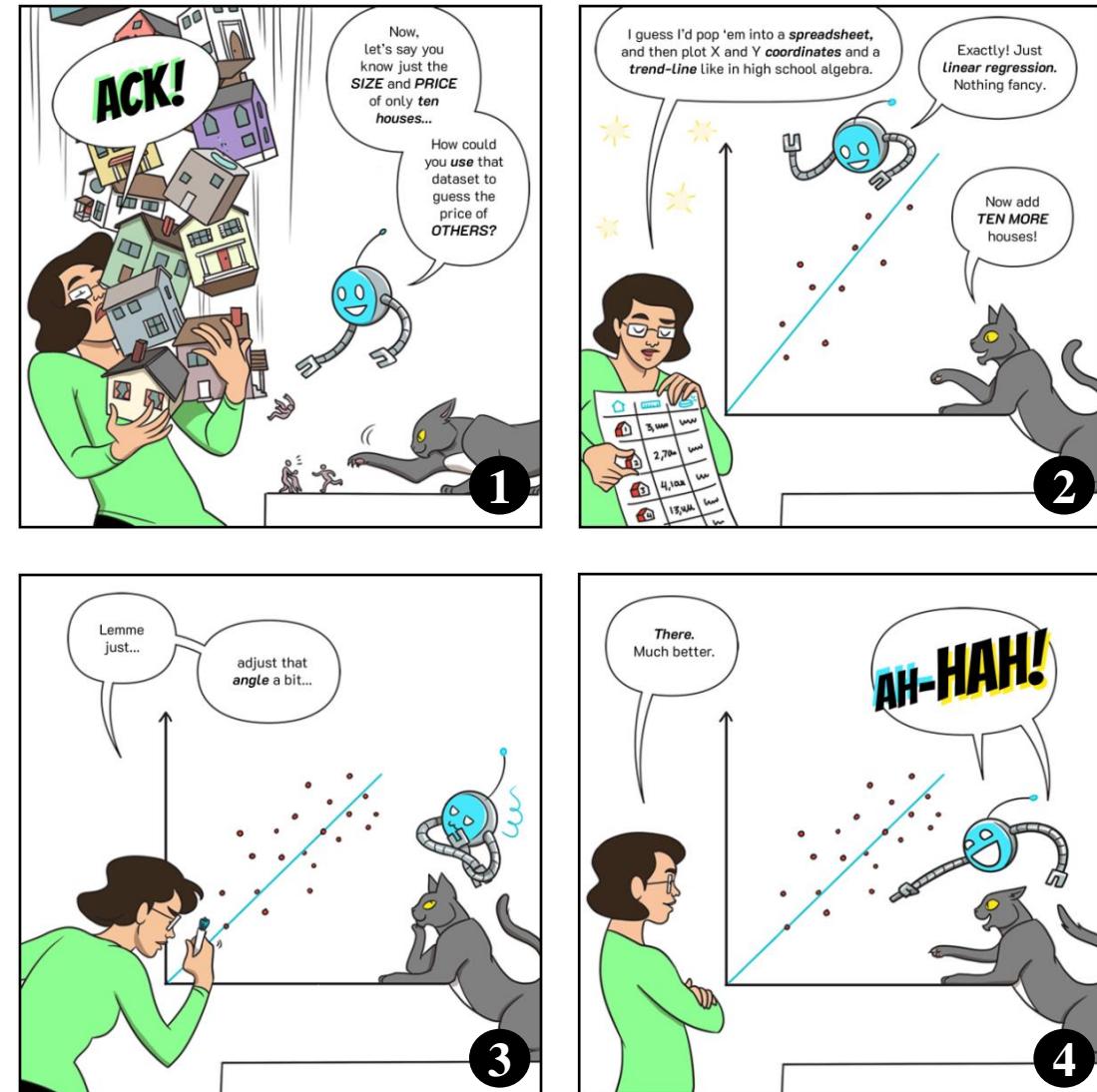


Classification: An intuition  
<https://cloud.google.com/products/ai/ml-comic-1>

# Task Of Machine Learning

## Regression

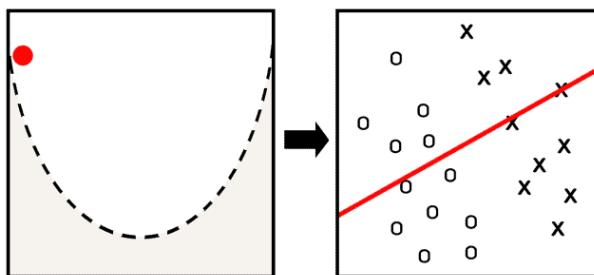
- How to predict the price of house based on its attribution?



# Task Of Machine Learning

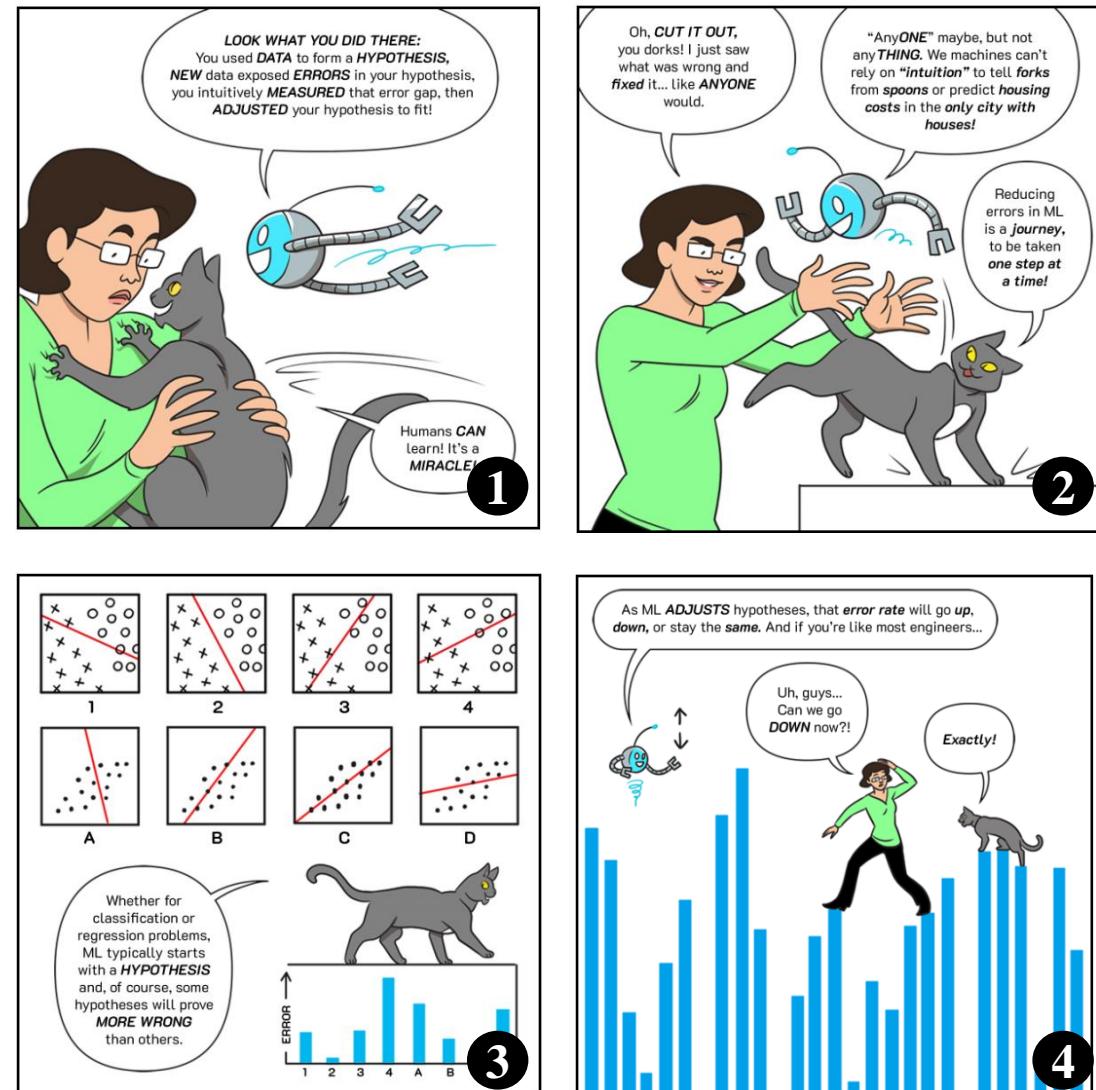
## Learning? Optimizing?

- What the basis for machine decision-making?
- Loss function : the measurement of difference between prediction and true value;
- With the help of optimizers, machine learning algorithms continuously reduce the value of the loss function, ultimately learning a 'line'.



← The Learning Process Of Machine

Machine “Learning”: An Intuition→  
<https://cloud.google.com/products/ai/ml-comic-1>



# General Steps Of Machine Learning

## General Steps

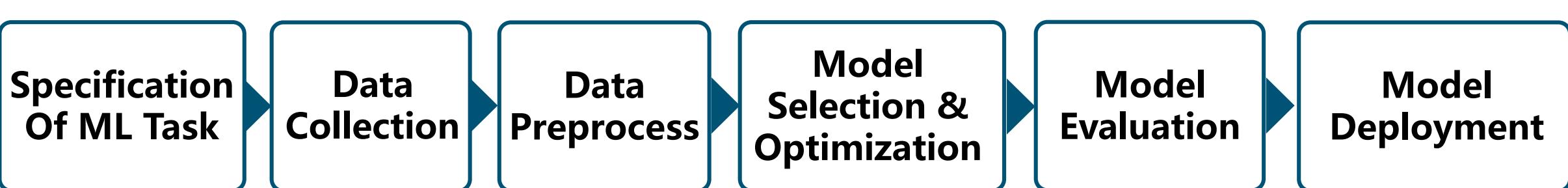
- Specification Of ML Task
- Data Collection
- Data Preprocess
- Model Selection
- Model Training
- Model Evaluation
- Model Deployment

## Classification

- Data Collection
  - Data Labeling
- Data Preprocess
- Model Selection & Training
  - KNN、Logistic Regression
- Classification Accuracy
- Model Deployment

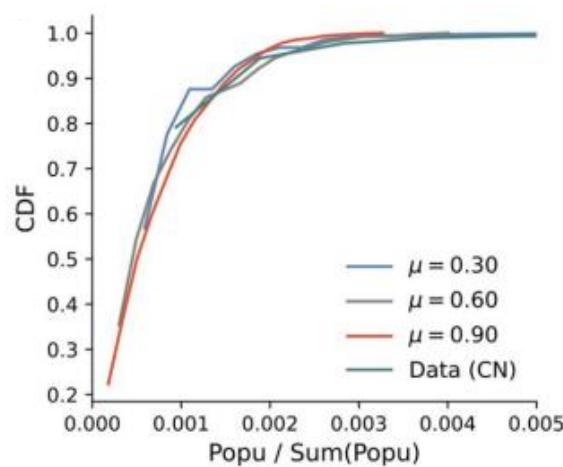
## Regression

- Data Collection
  - Explain & Response Variables
- Data Preprocess
- Model Selection & Training
  - Linear Regression
- Prediction accuracy
- Model Deployment

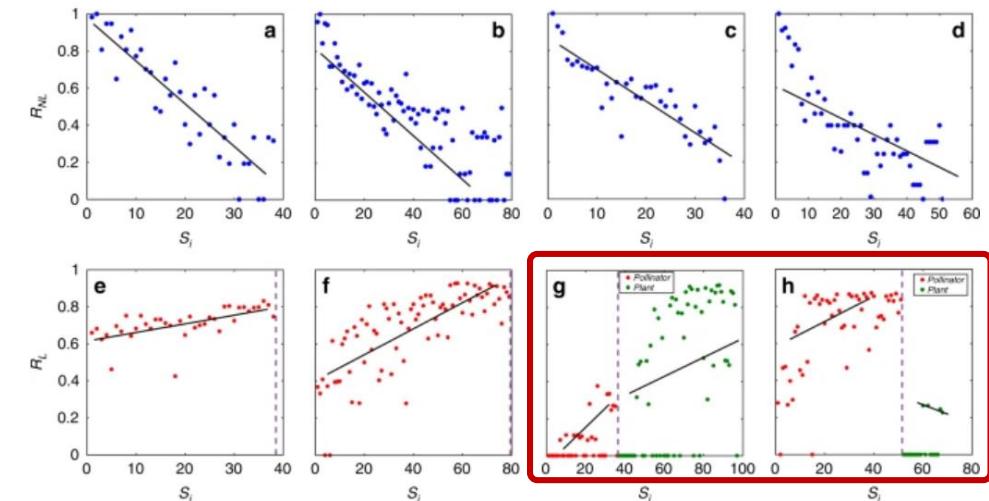
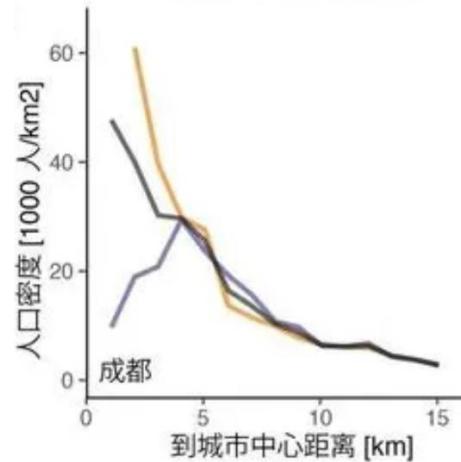


## Non-linear Relationship

- Machine learning algorithms ultimately learns a 'line'. **Fold Line? Curve?**



Curve of non-linear relationship in socio-economic phenomena

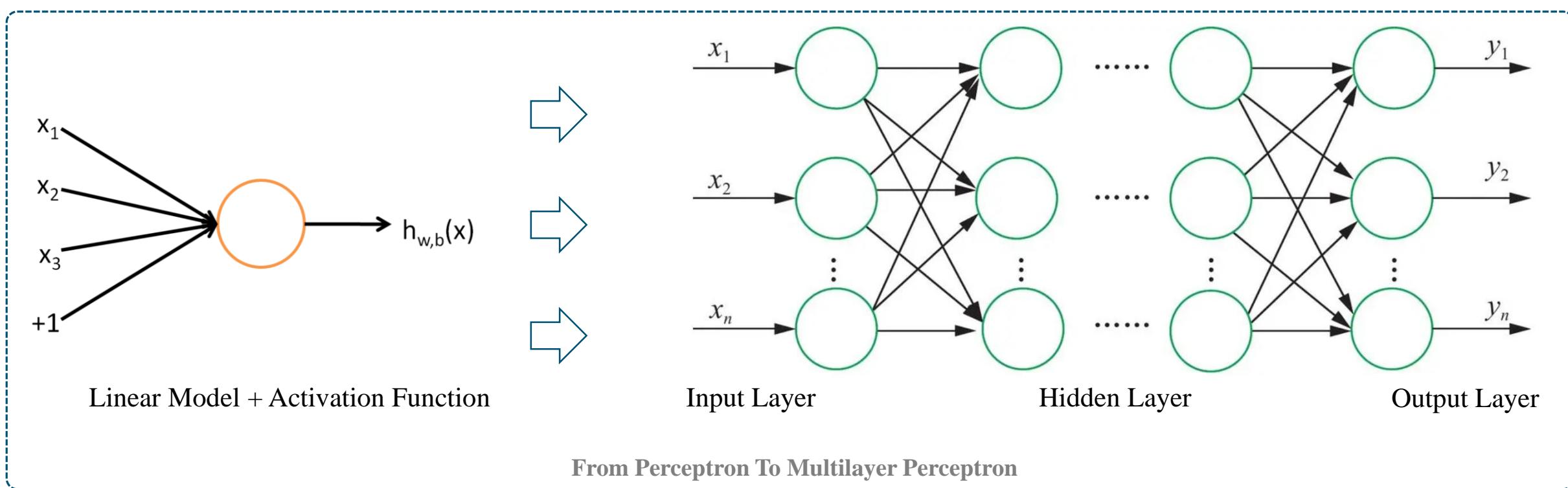


- Socio-economic phenomena exhibit intricate and non-linear characteristics;
- Traditional model cannot unravel the complex relationship between response and explain variables;
- The emergence of DL provides method to understand non-linear relationships.**

# Typical Models In Deep Learning

## Multilayer Perceptron, MLP

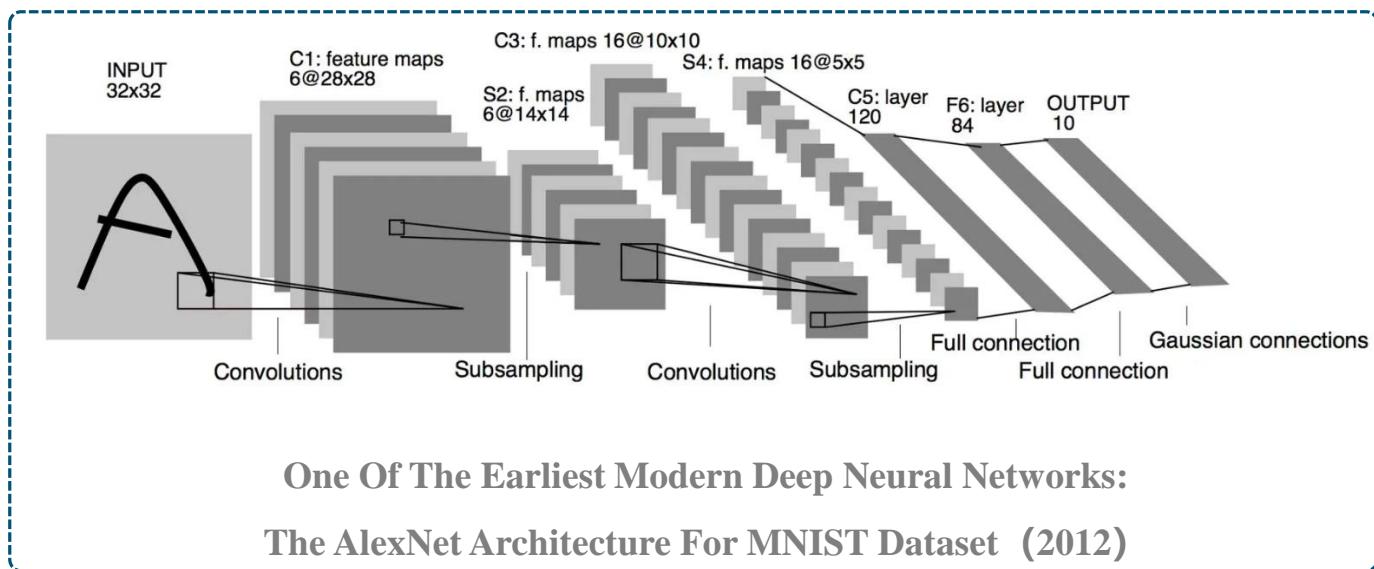
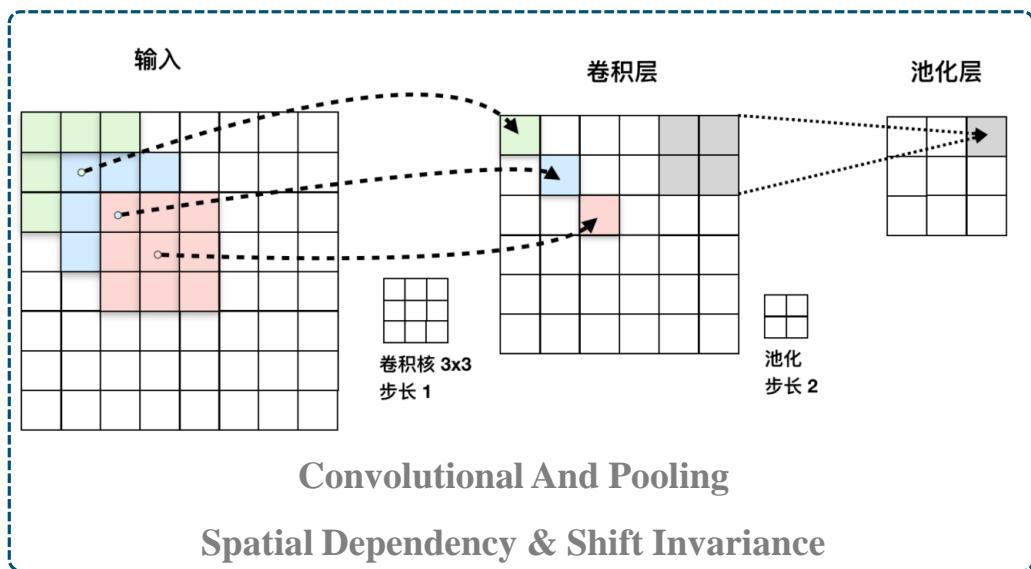
- Increasing the number of layers can enhance the model's ability.
- The activation function enables the model to learn nonlinear features in the data.



# Typical Models In Deep Learning

## Convolutional Neural Networks, CNN

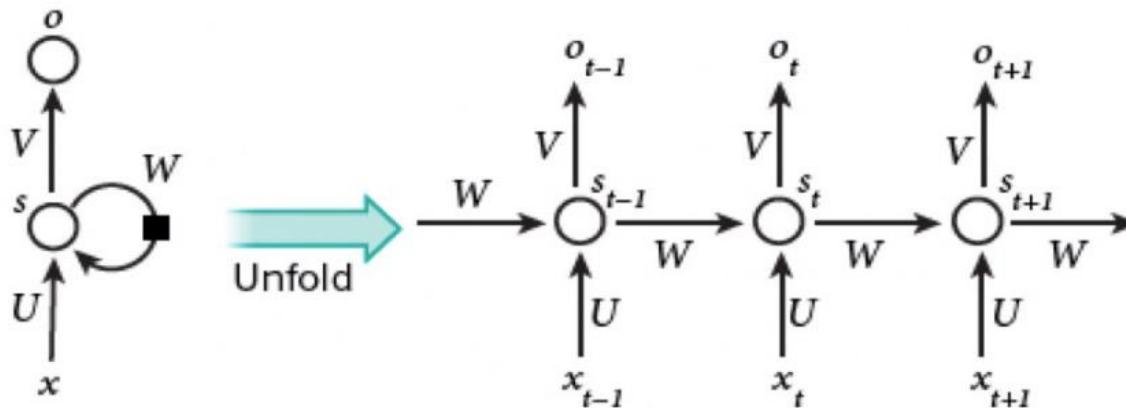
- CNNs are also known as **shift invariant or space invariant** artificial neural networks (SIANN). Based on the assumption of locality and translation invariance, CNNs provide translation-equivariant responses known as **feature maps**.
- CNNs is typically used in computer vision(CV) tasks: LeNet, AlexNet, UNet, ResNet, etc.



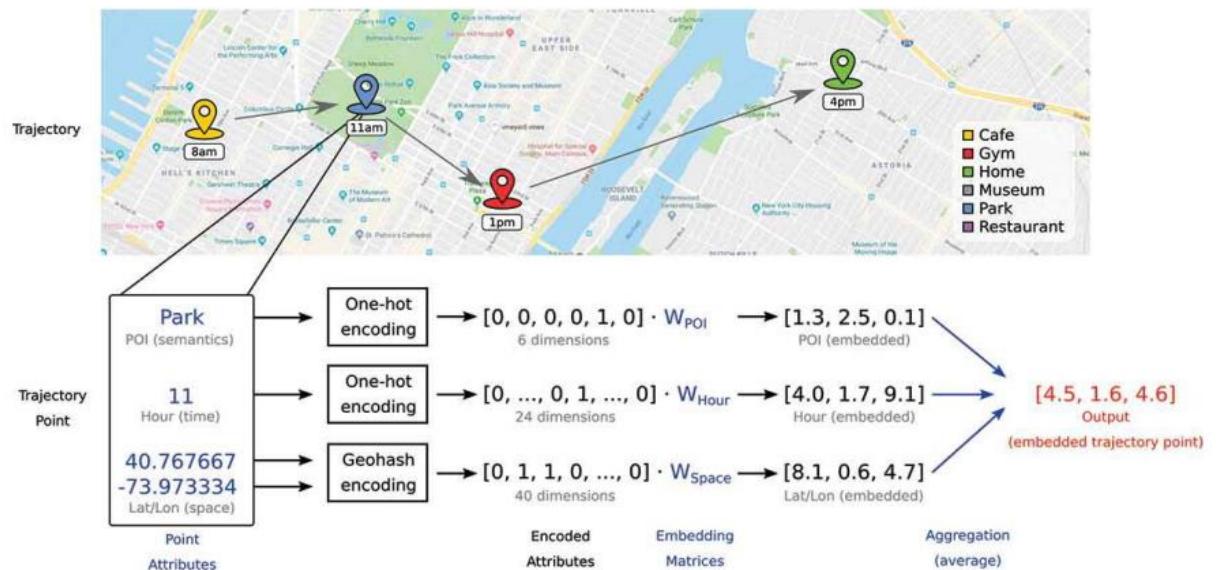
# Typical Models In Deep Learning

## Recurrent Neural Network, RNN

- Recurrent neural networks (RNNs) are a class of algorithms for sequential data processing;
  - RNN, LSTM, GRU etc.
- RNNs processes data across multiple time steps, making them well-adapted for modelling and processing text, trajectories, and time series.



The Principal Of RNN: Capture Temporal Dependency In Time Series



LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. *Nature*, 521(7553), 436-444.

May Petry, L., Leite Da Silva, C., Esuli, A., Renso, C., & Bogorny, V. (2020). MARC: a robust method for multiple-aspect trajectory classification via space, time, and semantic embeddings. *International Journal of Geographical Information Science*, 34(7), 1428-1450.

# Typical Models In Deep Learning

## Transformer

- Core: Attention

- Key Structure

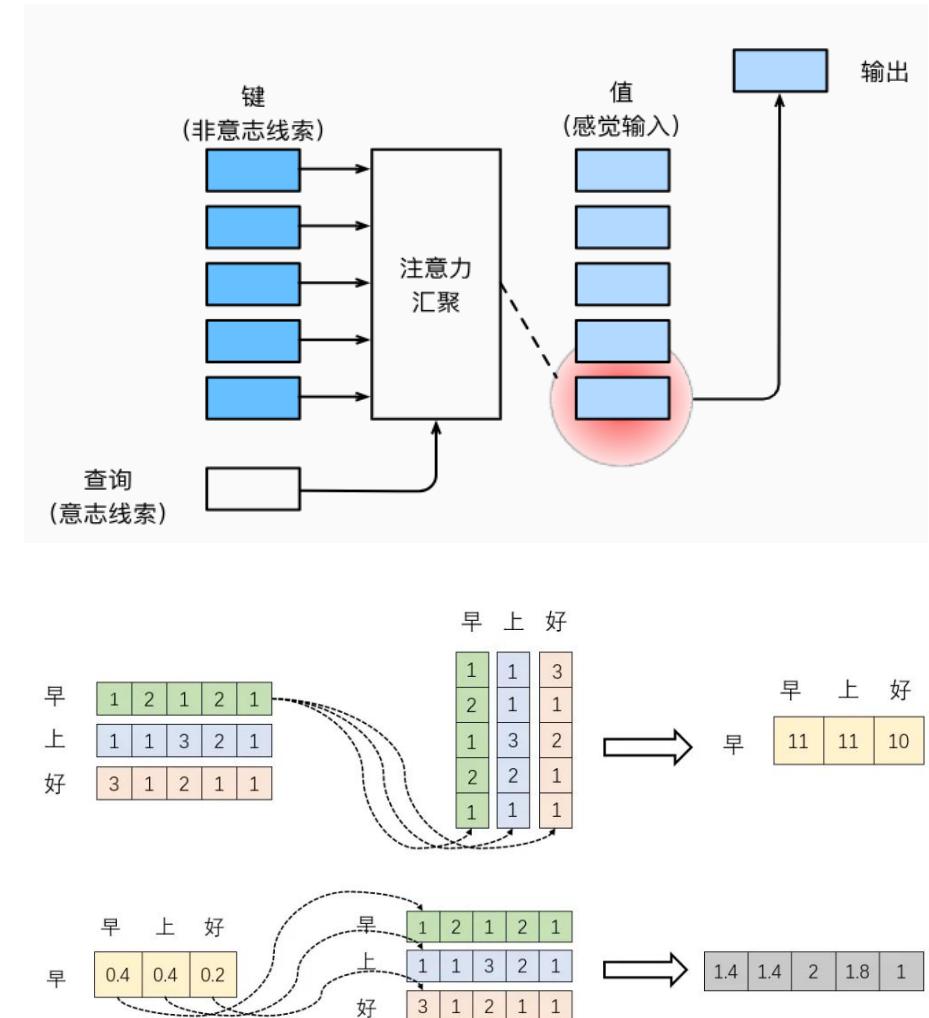
- Embedding: Constant and dense vector, represents the location and information of the trajectory points.

- Query & Key: Measure the relationship between trajectory points;

- Value: Obtaining most suitable values based on keys.

- Output : Numerical Representation, known as Embedding.

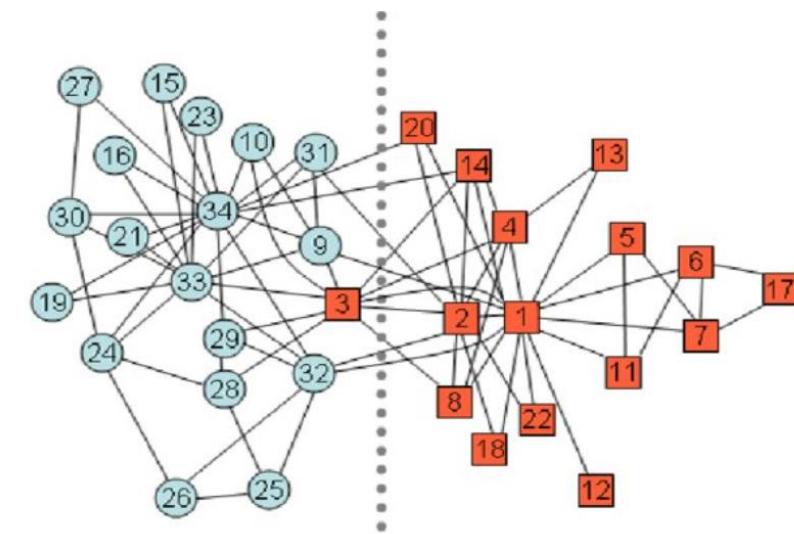
Attention Mechanism: An Example→



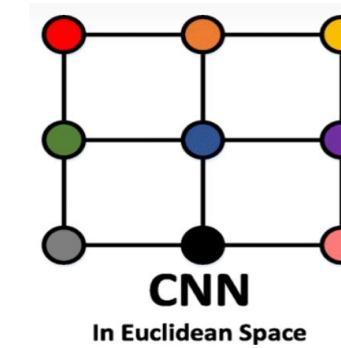
# Typical Models In Deep Learning

## Graph Neural Network, GNN

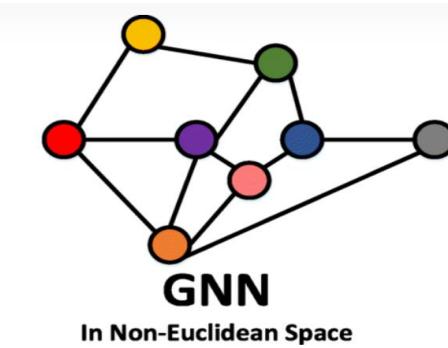
- A graph neural network (GNN) belongs to a class of artificial neural networks for processing data that can be represented as graphs (**Node-Link**).
- The key design element of GNNs is the use of **pairwise message passing**, such that graph nodes iteratively update their representations by exchanging information with their neighbors.
- In the more general subject of “geometric deep learning”, certain existing neural network architectures can be interpreted as GNNs operating on suitably defined graphs.



The Classical Example Of Social Network Analysis  
Zachary's Karate Club



**CNN**  
In Euclidean Space

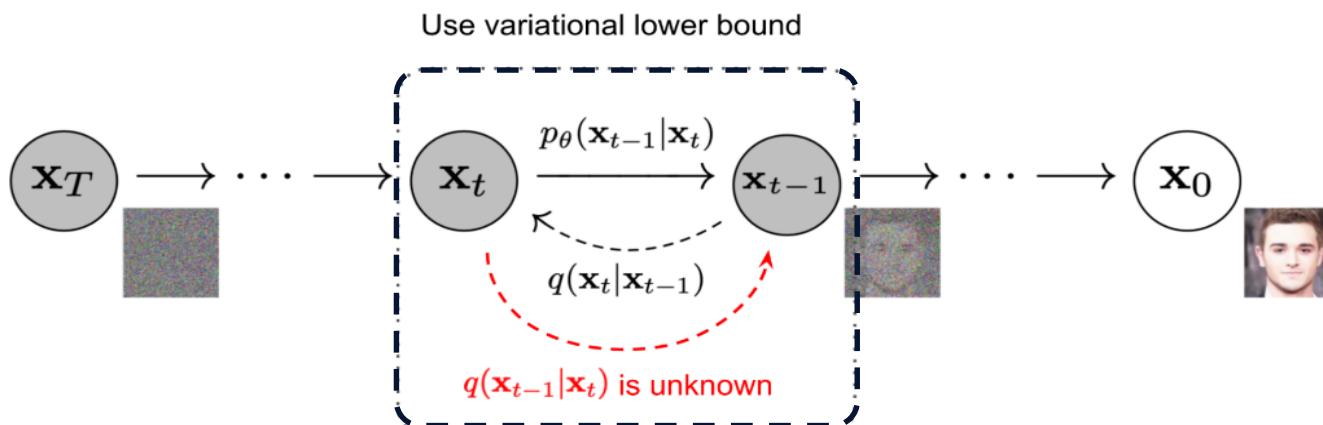


**GNN**  
In Non-Euclidean Space

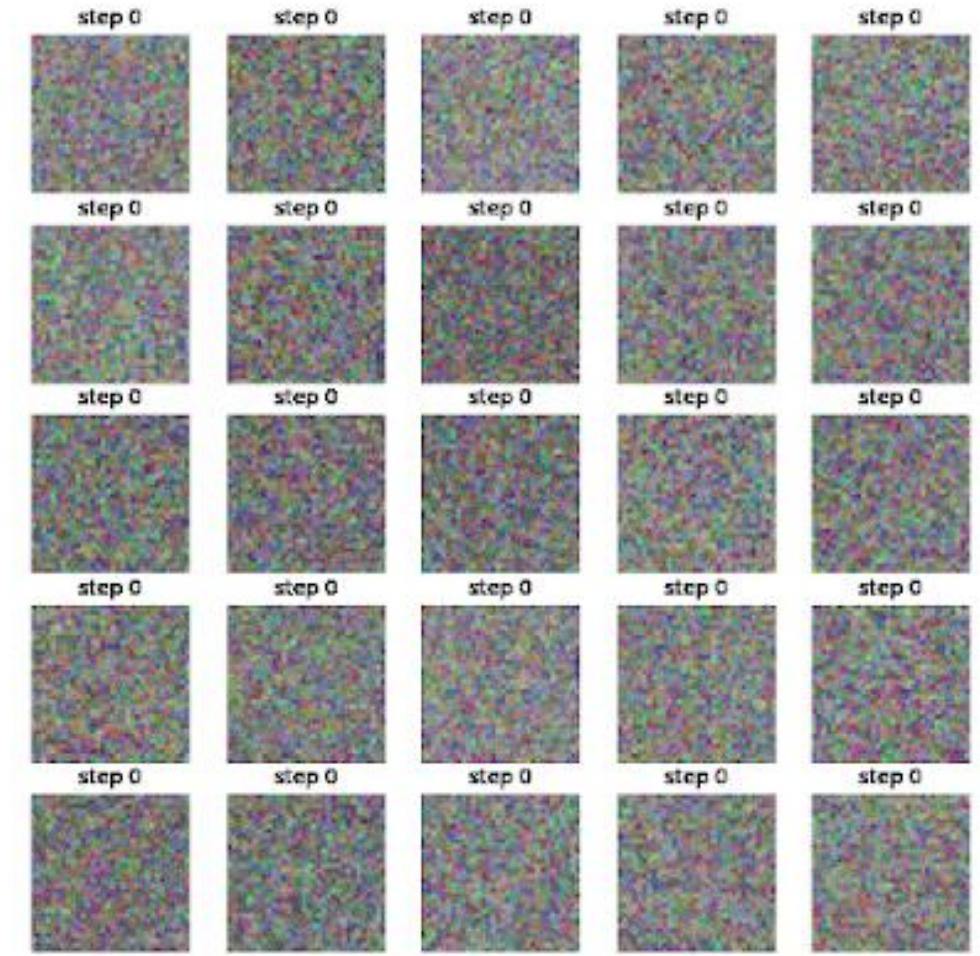
# Typical Models In Deep Learning

## Generative Models

- Learn the distribution of the data itself:
  - GAN, VAE, Diffusion Model, etc.
- Generative models are usually used in topics such as trajectory generation and plan generation in urban science.



The Principle of Diffusion Model: the forward process, and the reverse process



Diffusion Model: An Intuition Presented In GIF

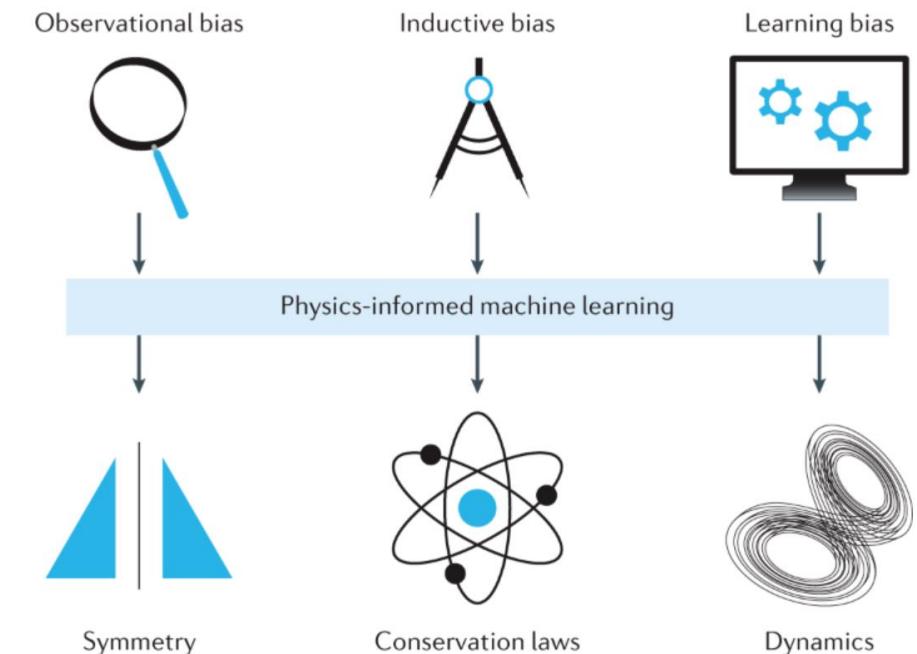
## Data-driven methods perform poor in specific domains

- **Solution:** Integrate prior knowledge based on empirical understanding of and mathematical principles.
- The PINN is one of the outstanding algorithms that can provide valuable insights for integrating prior knowledge into AI to address urban social issues.

## Physics-Informed Neural Networks (PINN)

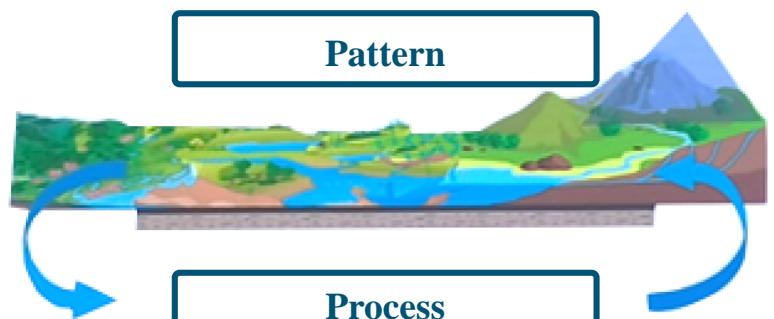
- By adding the difference between the physics equations before and after iteration loss function, the training results conform to physical laws.

The Principle Of Integrating  
Physical Knowledge And ML



## Geospatial Artificial Intelligence, GeoAI

- GeoAI is the achievement of integrating geographical prior knowledge and AI algorithms.
- The purpose of GeoAI is to support the **data-intensive scientific discovery** in geographical science.



$$Y = f(x)$$

Spatial-temporal Analysis Model

## How to combine the understanding of geospatial big data with AI?

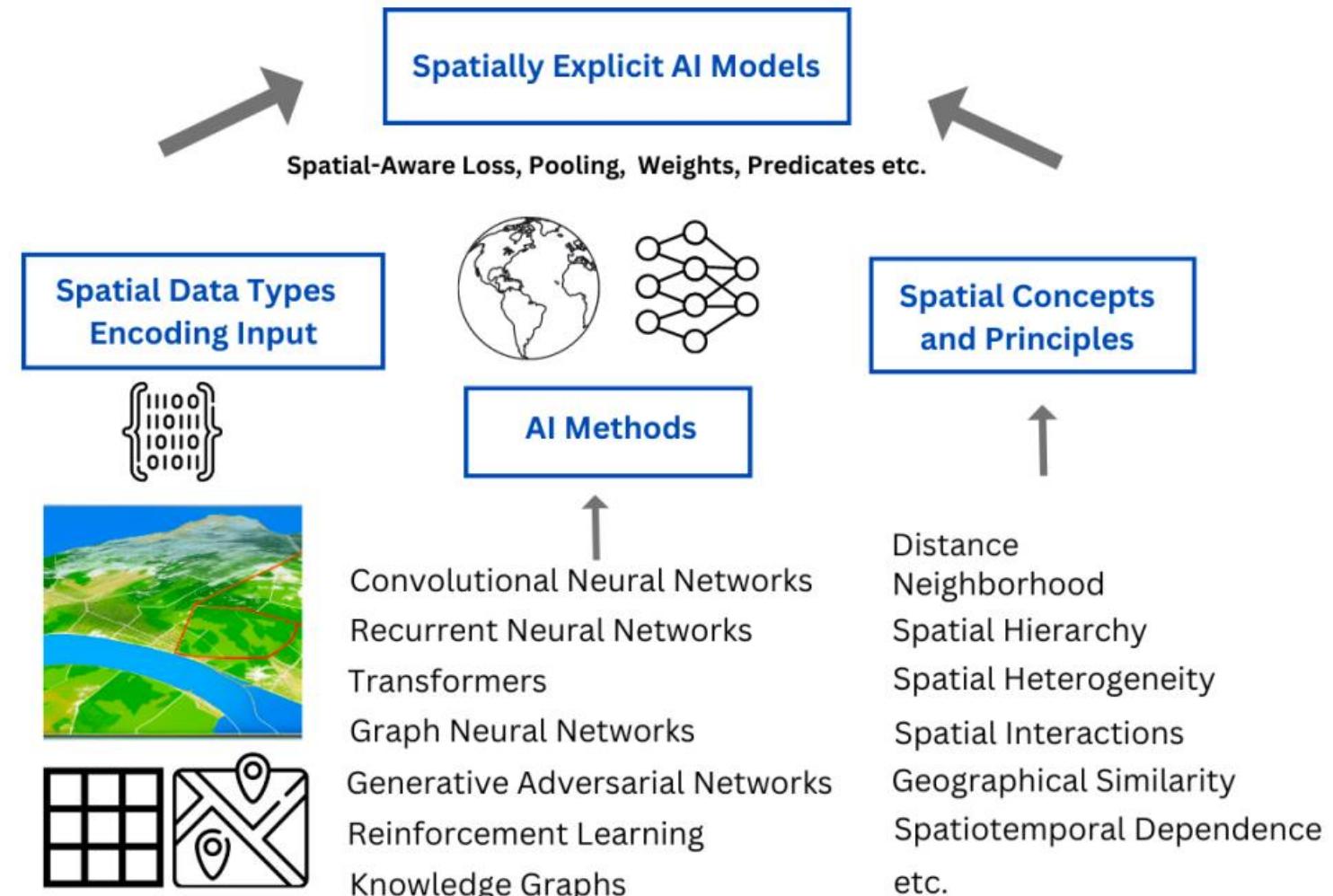
- The prosperity in AI techniques provides methodologies to understand and model urban phenomena for researchers.
  - Spatial Relationship And Spatial Autocorrelation: **CNN**;
  - Time-series Dependence: **RNN, LSTM, Transformer**;
  - Graph Data Structure: **GNN, GCN**;
  - Simulation And Generation: **GAN, VAE, Diffusion Model**;
  - Agent: **Reinforcement Learning, RL**.
- How to combine the modeling methodologies mentioned above with geographical knowledge?
  - **Spatial Explicit Artificial Intelligence**

# Spatial Explicit AI

## Test for Spatial Explicit AI

- Invariance Test
- A spatially explicit model is **not invariant** under relocation.

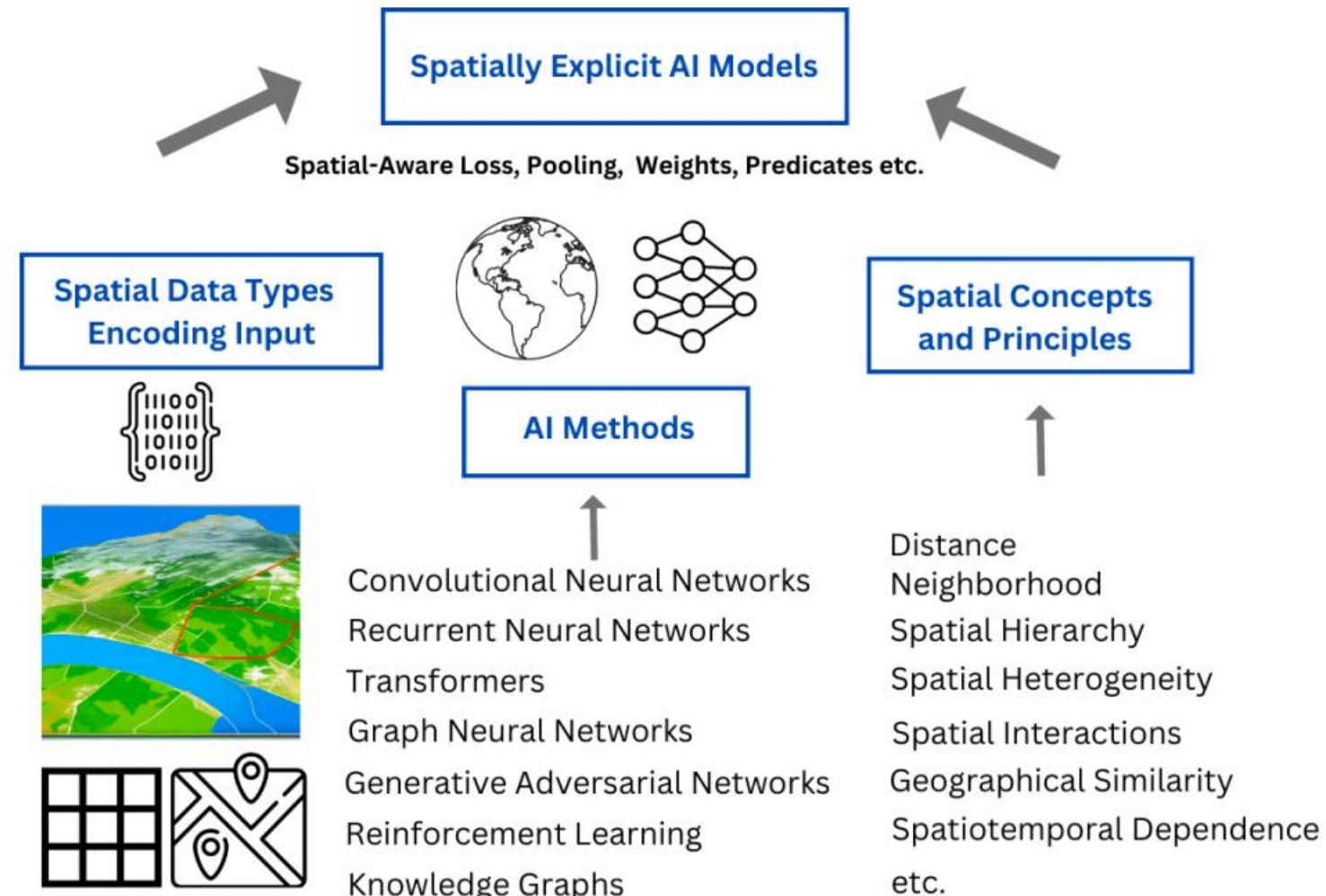
- Representation Test
- A spatially explicit model includes **spatial representations** such as coordinates, spatial relations, etc. in its implementations.



# Spatial Explicit AI

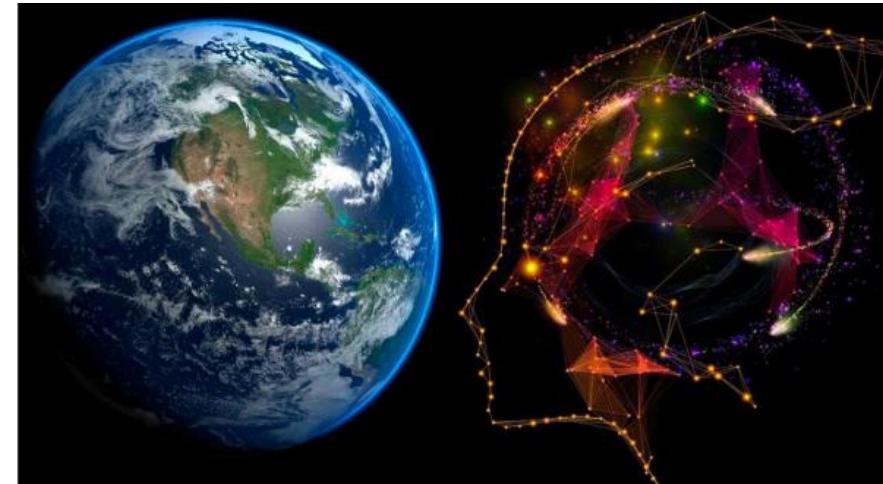
## Test for Spatial Explicit AI

- **Formulation Test**
- A spatially explicit model includes **spatial concepts** in their **formulation** such as spatial neighborhoods, etc.
  
- **Outcome Test**
- The spatial structures of spatially explicit models' inputs and outputs are different.



## What is the vision for developing GeoAI?

- **Cognitive** : Understand human cognitive system and decision-making process.
- **Engineering** : Develop computer programs that have capabilities for understanding, processing, and generating human-like intelligence



## What are the advantages of GeoAI?

- **Convenient Data Representation**: capable of handling various types of data ;
- **Spatial Dependence Priors**: explicitly incorporate spatial effects such as neighborhood variation, related structures, and distance decay into the design of the model;
- **Flexible Model Assumptions**
- **Capability Of Predicting And Explaining The Unknown.**

# **Applications Of GeoAI In Urban Science**

# Outline

- Spatial Representation Learning
- Spatial Interpolation And Prediction Methods
- Explainability In GeoAI
- Spatial Cross Validation

# Representation Learning In GeoAI

## Spatial Representation Learning In GeoAI

### □ Data Extraction

#### □ Traditional Topics

- What Characteristics Can Facilitate Car Recognition By Programs?
- How to predict houses' price according to their attributes?

#### □ Solution: Designing Artificial Features→Representation Learning

- Extracting Characteristics From Data Automatically;
- **Result:** High-Dimensional, Constant Dense Vector;
- The Results Can be Input Into Downstream Tasks Such As Classification, Regression etc.

**Spatial-temporal Data Requires Methods Different From Traditional Representation Learning.**

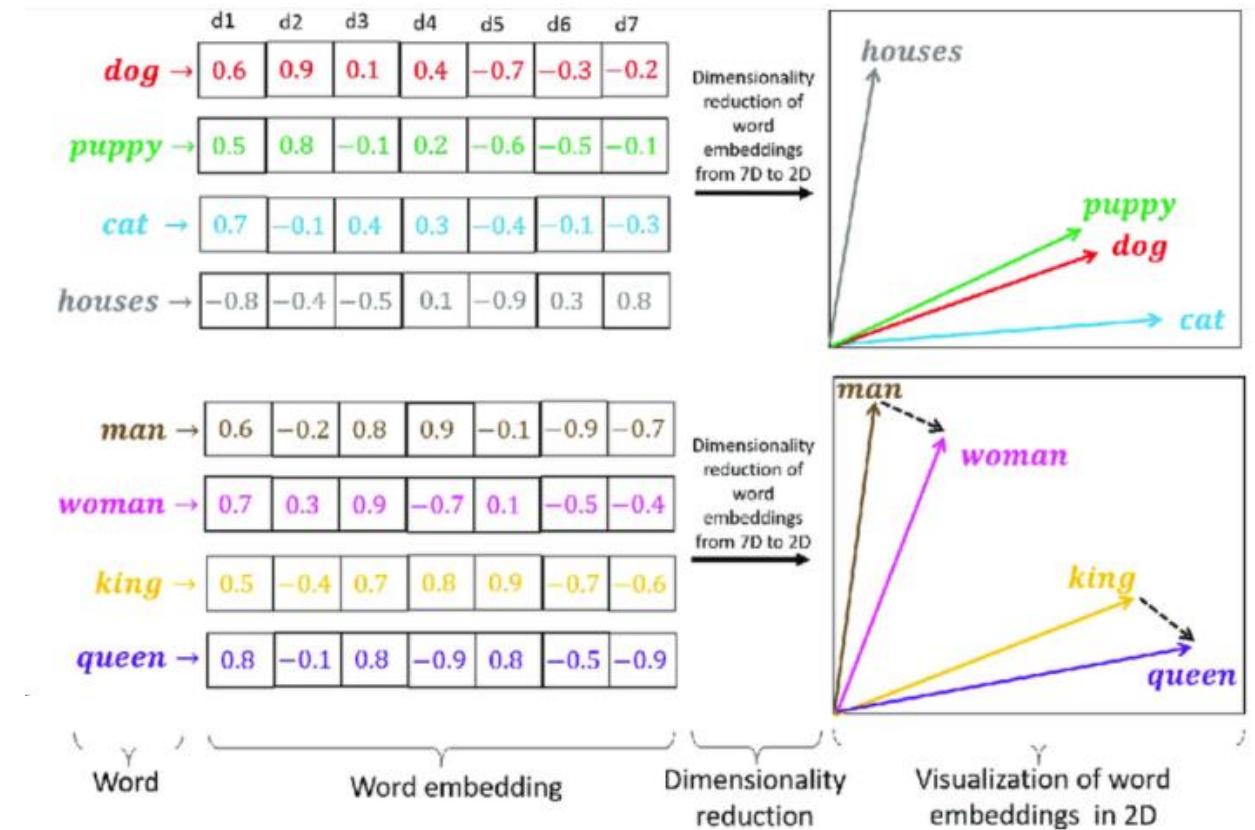
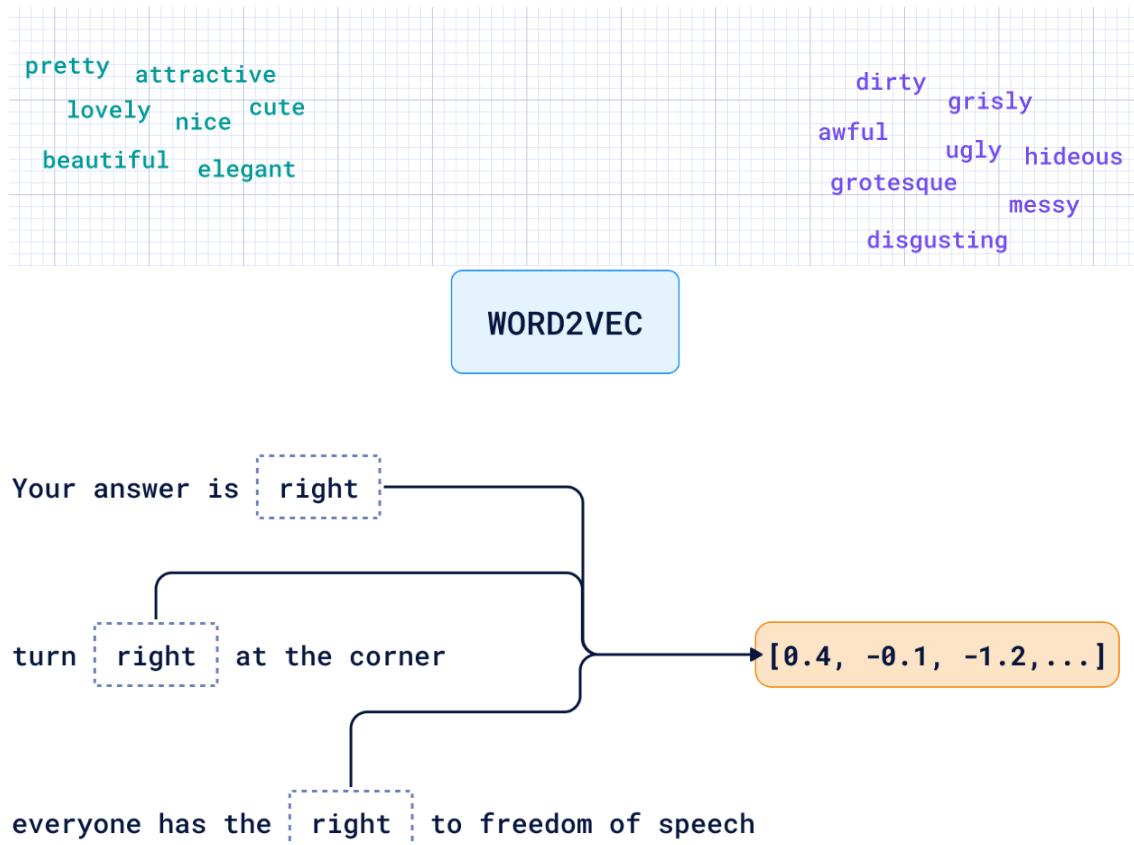


The One-hot Encoding Of Abandon In CET6. The Result Vector Can Be Interpreted As The Location In Dictionary.

Every Vocabulary Can Be Represented To Unique Vector

# Representation Learning In GeoAI

## Representation Learning: An Intuition



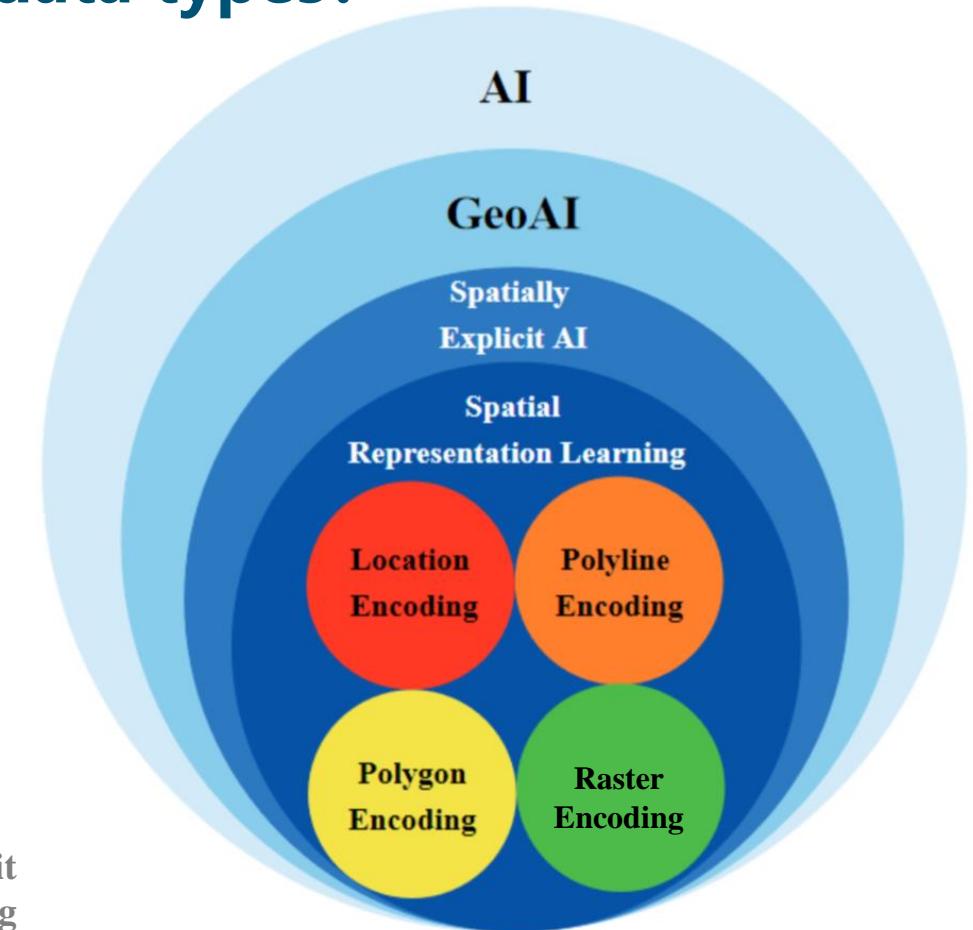
Embed the sentence into a dense vector

Cosine similarity is a measure of the degree of the difference between embeddings

# Representation Learning In GeoAI

## Spatial Representation Learning on various data types:

- Location Encoding
- Polyline Encoding
- Polygon Encoding
- Spatial Representation Learning On Raster
- Spatial representation learning on irregular objects



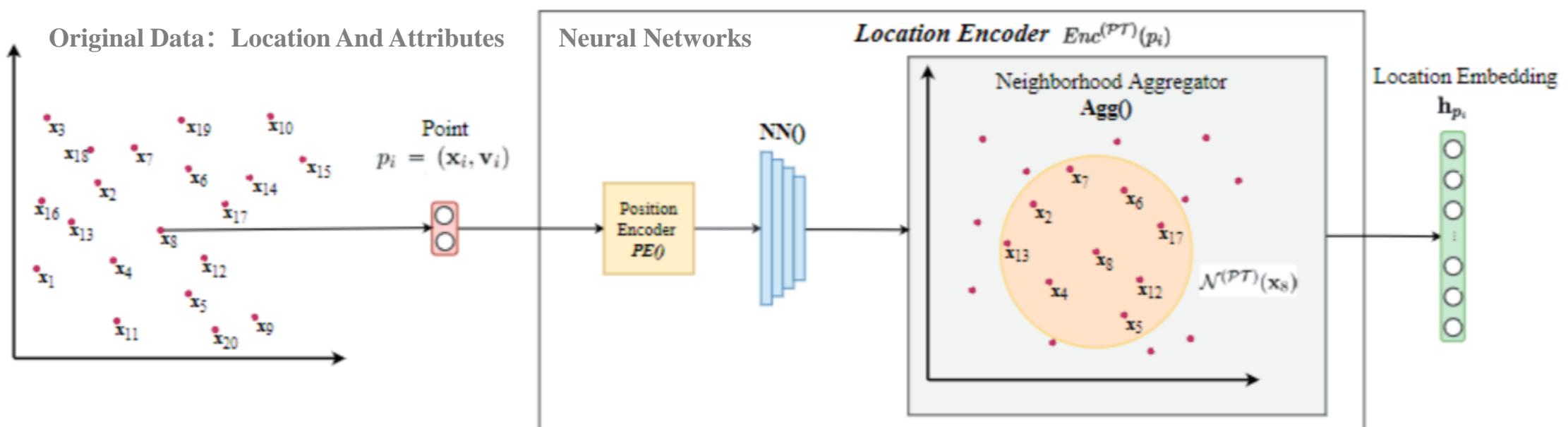
The Relationship Between AI, GeoAI, Spatially Explicit  
AI And Spatial Representation Learning

# Location Encoding

## Location Encoding: How To Make Algorithms Recognize Point Data?

- There is no information loss since the point-to-grid process is skipped and MAUP is avoided.
- It is widely used in process of 3D point cloud and estimation of geographical distribution.
- CNNs are commonly employed for location encoding to capture spatial dependency within data.

### □ Distance Preservation & Direction Awareness



The General Steps Of Location Encoding In GeoAI: Embed Location And Attributes Into Vectors Using Neural Networks

# Location Encoding

## Location Encoding:

### □ Single Point Location Encoders

#### □ Discretization-based location encoder

Discrete Points To Spatial Fishnet + One hot;

#### □ Direct Location Encoder

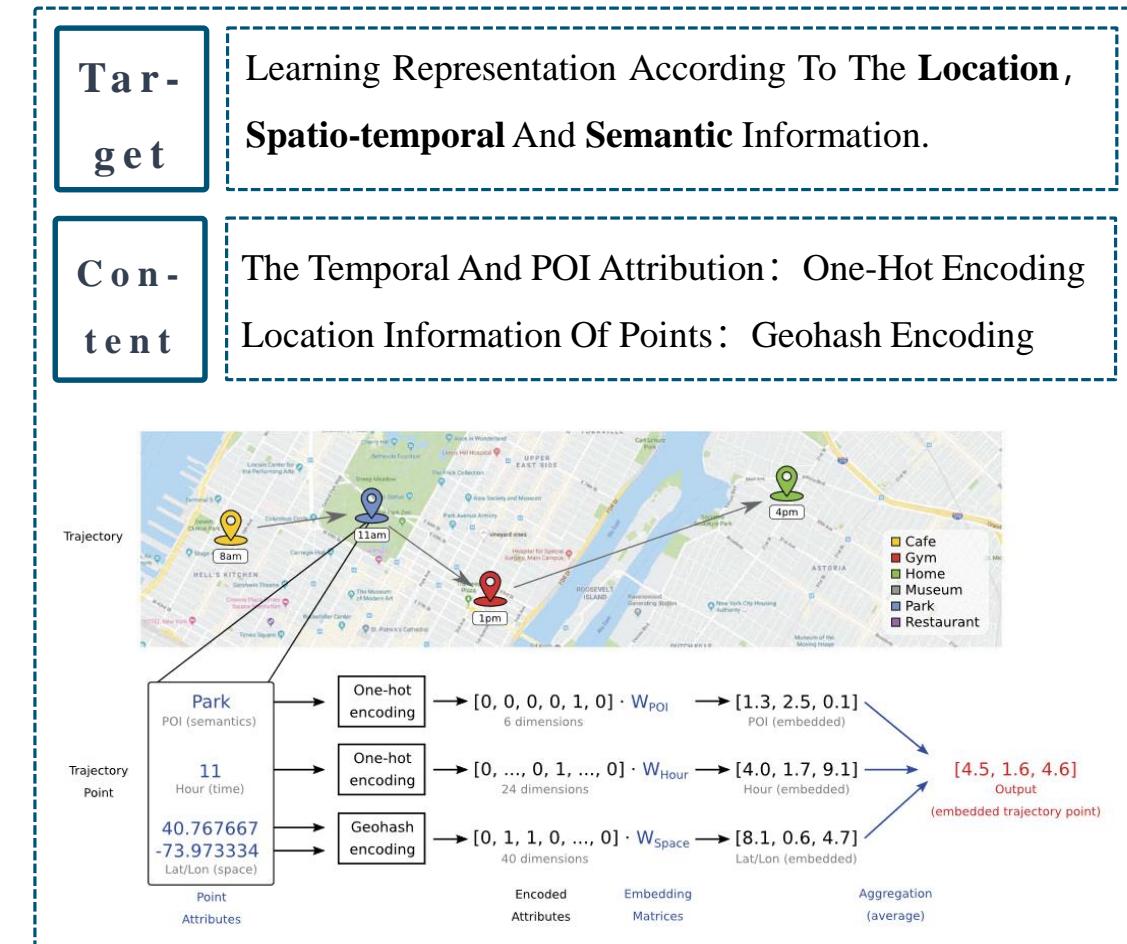
Standardize The Longitude & Latitude

#### □ Transformer-Based Location Encoder

### □ Aggregation Location Encoders

#### □ Global Aggregation Location Encoder

#### □ Local Aggregation Location Encoder



Mai, G., Janowicz, K., Hu, Y., Gao, S., Yan, B., Zhu, R., Cai, L., & Lao, N. (2021). A Review of Location Encoding for GeoAI: Methods and Applications. arXiv.Org. <https://doi.org/10.1080/13658816.2021.2004602>

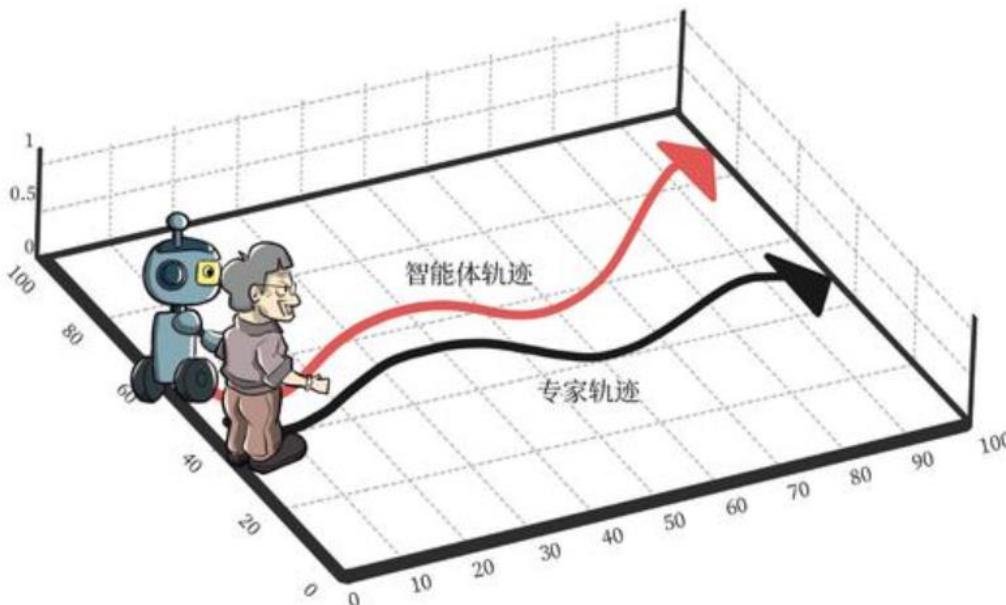
May Petry, L., Leite Da Silva, C., Esuli, A., Renso, C., & Bogorny, V. (2020). MARC: a robust method for multiple-aspect trajectory classification via space, time, and semantic embeddings. International Journal of Geographical Information Science, 34(7), 1428-1450.

# Polyline Encoding

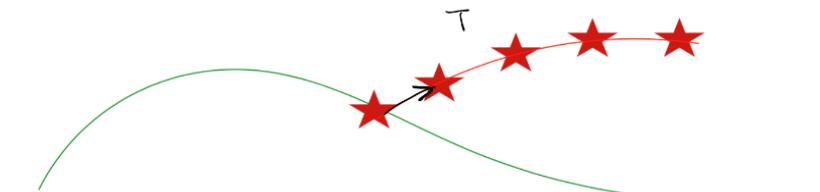
## Why Polyline Encoding?

Is it feasible to concatenate the embeddings of locations merely as representations of polyline?

- Indefinite Length ;
- Spatio-temporal Dependence.



Problem: Compounding Errors



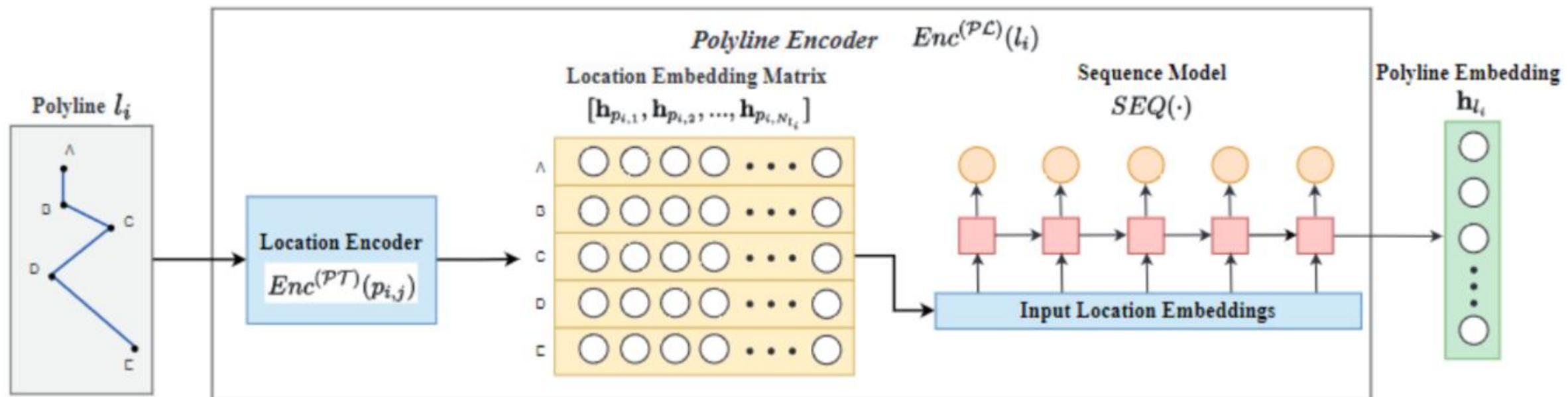
$$\text{Error at time } t \text{ with probability } \epsilon \\ \mathbb{E}[\text{Total errors}] \leq \epsilon(T + (T - 1) + (T - 2) \dots + 1) \propto \underline{\epsilon T^2}$$

Take Imitation Learning As An Example, Compounding Errors Can Easily Lead Autonomous Vehicles Astray From The Correct Path.

# Polyline Encoding

## Polyline Encoding: How To Make Algorithms Recognize Polyline Data?

- Polyline can be directly represented as high-dimensional embedding through a neural network.
  - Polyline are usually regarded as set of points with temporal information.
- RNNs are commonly employed for polyline encoding to capture temporal dependency within data.

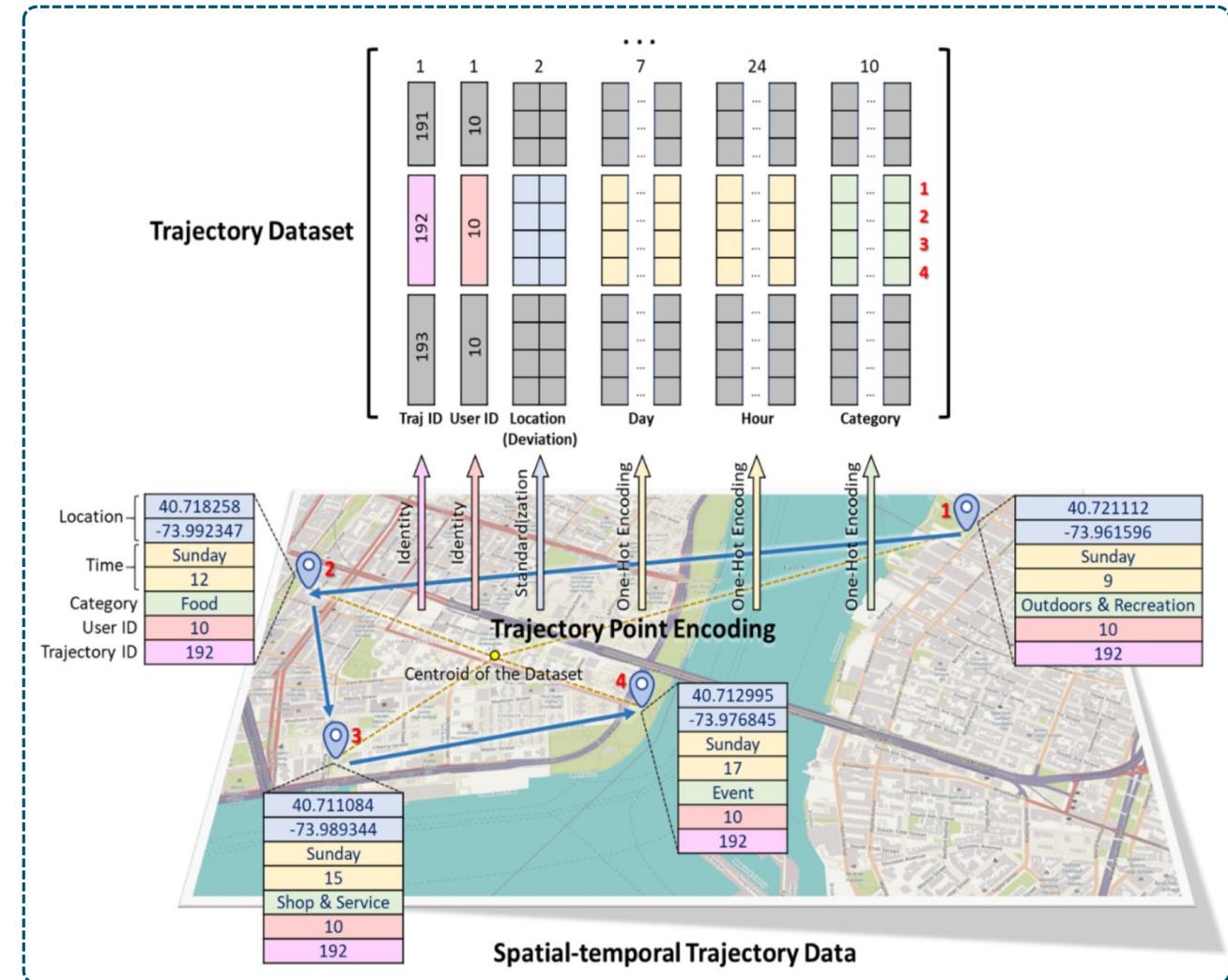


GeoAI 中对多段线进行编码的一般流程：采用神经网络架构将多段线直接表示为高维嵌入，一般包含顶点嵌入与位置嵌入两个步骤。

# Polyline Encoding

## Case Study Of Location Encoding

- Convert Trajectory ID, User ID, Location, Date and other attributes to numeral values.
- Concatenate the result of conversion to feature vectors as encodings of trajectory points.



Trajectory Embedding: An Intuition (Rao et.al, 2020)

# Polyline Encoding

## Research Target

- Standardize Trajectory Without Loss Information.
- Encoding the heterogeneous dimensions associated to each trajectory point;

## Research Content

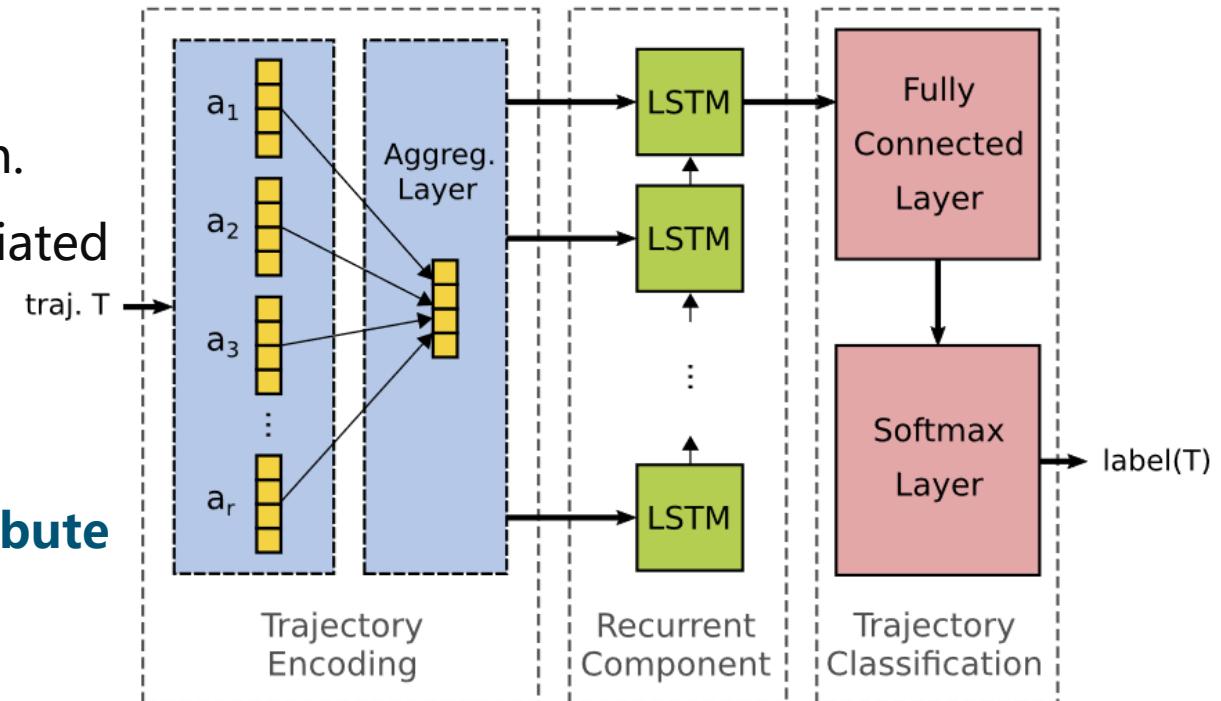
- Classify multi-aspect trajectory based on **attribute embedding** and **RNNs**.

## Methodology

- Employing LSTM to capture sequential patterns;

## Result

- **Trajectory Classification:** behaviors, travel patterns.

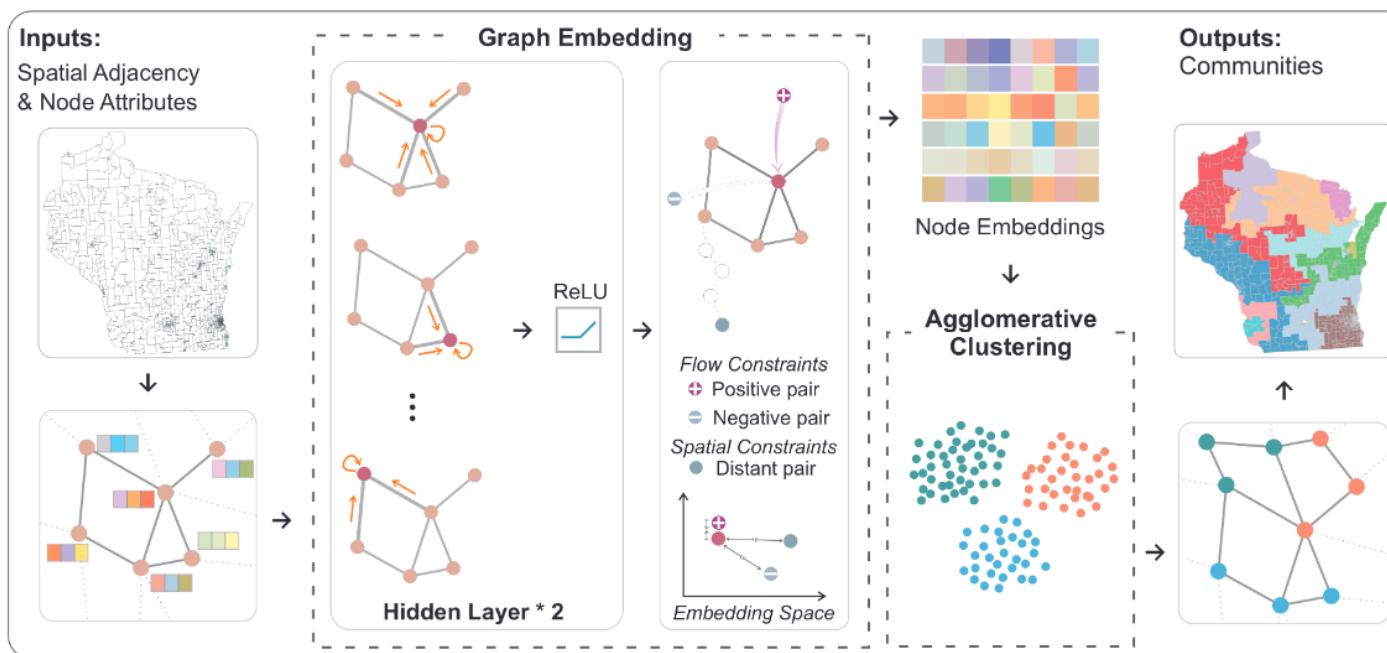


Trajectory Embedding: An Intuition (May et.al, 2020)

# Polygon Encoding

## Research Target

- The specificity of spatial networks: geospatial structure within graph, planar graph etc.
- Community detection algorithm on spatial networks based on GNNs : **Region2Vec**;
- Incorporate **Geographic Constraint** into the design of loss function: spatial neighborhood etc.



$$L_{hops} = \sum \frac{\mathbb{I}(hop_{ij} > \epsilon) d_{ij}}{\log(hop_{ij})}; Loss = \frac{\sum_{p=1}^{N_{pos}} \log(s_p) d_{posp} / N_{pos}}{\sum_{q=1}^{N_{neg}} d_{negq} / N_{neg} + L_{hops}}, \quad (2)$$

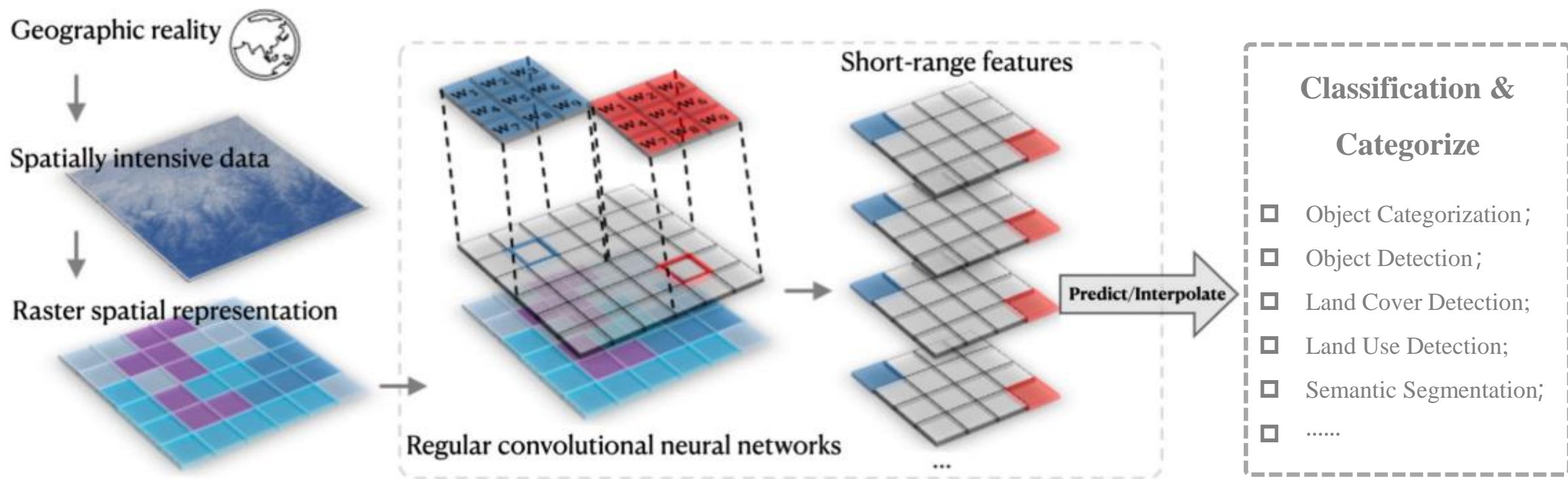
where  $hop_{ij}$  represents the hop numbers of the shortest path between  $v_i$  and  $v_j$  in the graph, and  $d_{ij}$  is the euclidean distance between the corresponding embedding representations.  $\mathbb{I}(\cdot)$  is set to 1 if  $hop_{ij} > \epsilon$ , or 0 otherwise. Positive pairs and negative pairs of nodes are denoted by  $pos_p, p \in [0, N_{pos}]$  and  $pos_q, q \in [0, N_{neg}]$ , respectively. Since the intensity of flow  $s_p$  has a large range of values, we adopt a log transformation so that the flow values will not get overwhelmed by the extremely large values. The pseudo

## The Loss Function Of Community Detection

# Representation Learning On Raster

## Raster Representation: How To Make Algorithms Recognize Raster?

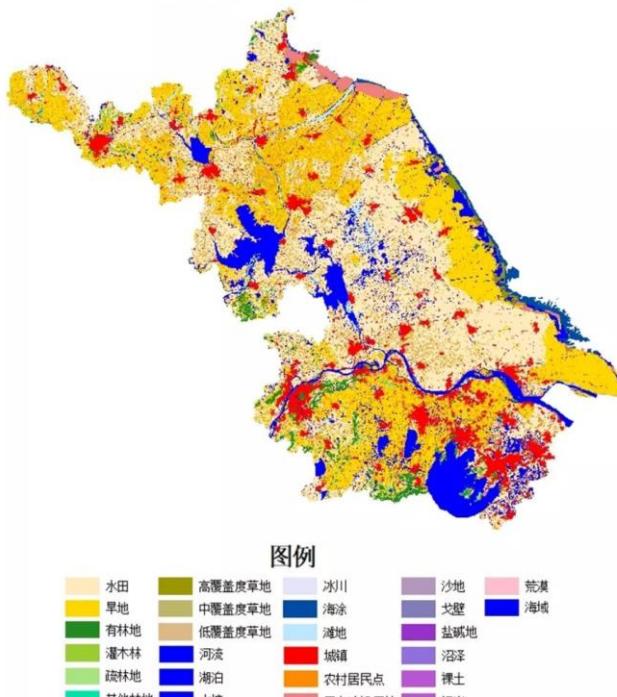
- Employ CNNs to get insights on deep spatial features in raster data.



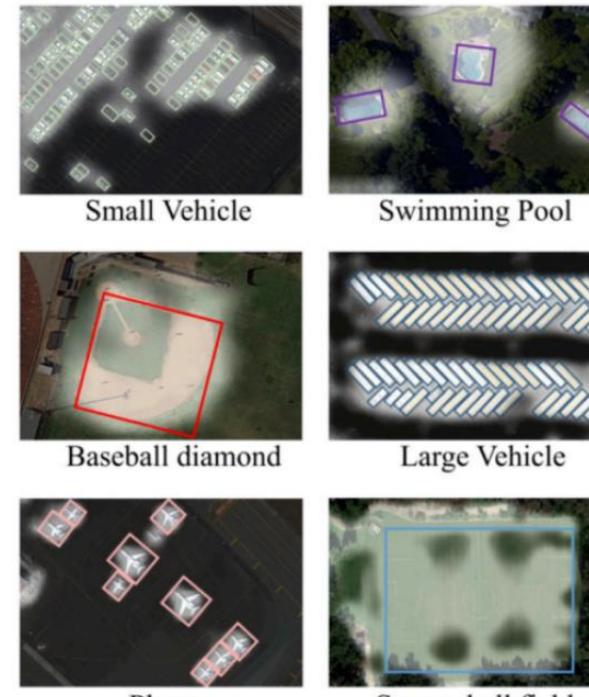
# Representation Learning On Raster

## Raster Representation

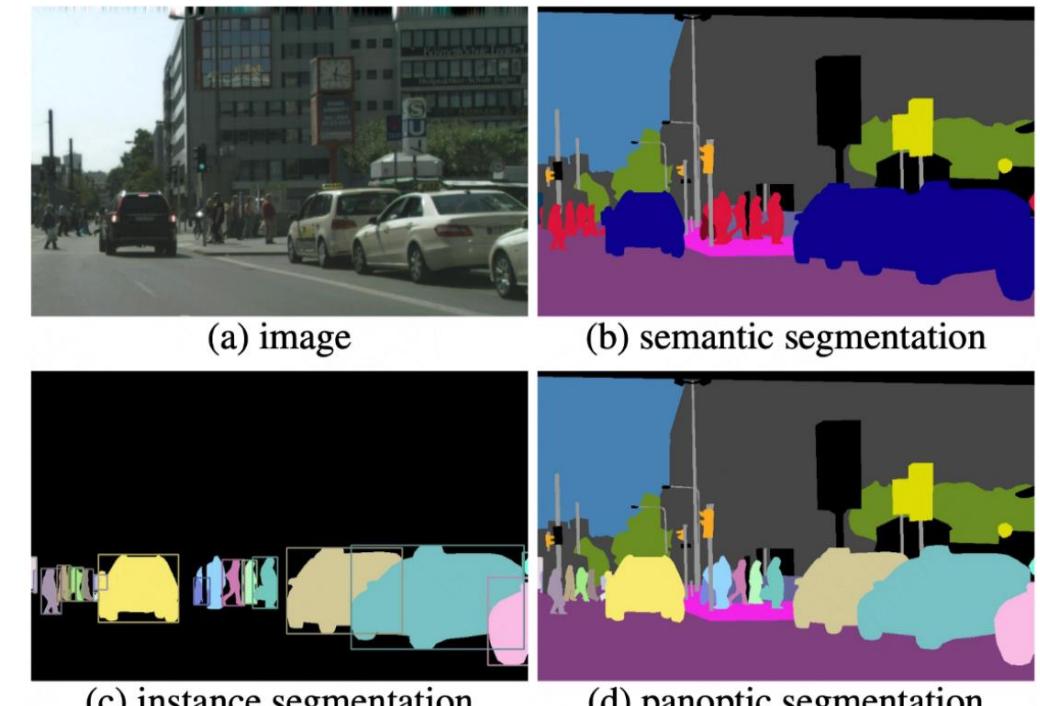
- The results of raster representation can be inputs of downstream tasks such as classification. Therefore, raster representation is commonly regarded as the sub-task of computer vision.



Land Cover Categorization



Remote Sensing Object Detection



Semantic Segmentation In Street View Image

# Representation Learning On Raster

## Research Intuition

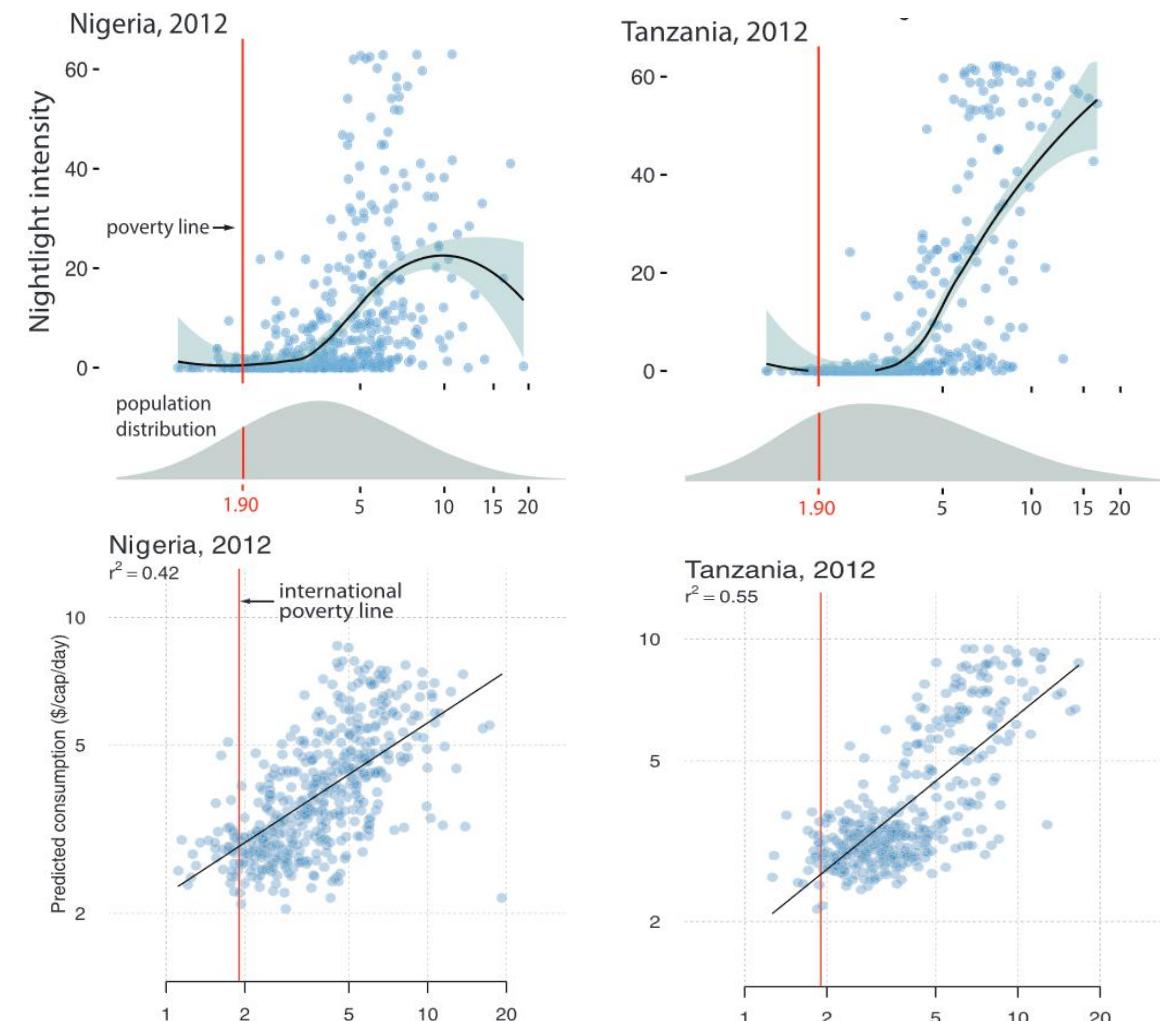
- ❑ Nightlights potentially less useful for studying and tracking the livelihoods of the very poor;
- ❑ LBS data relies on proprietary data sets.

## Research Content

- ❑ Propose a framework to make predictions about the spatial distribution of economic well-being using deep learning model.

## Methodology

- ❑ Train ridge regression model using daytime imagery features extracted by CNNs.

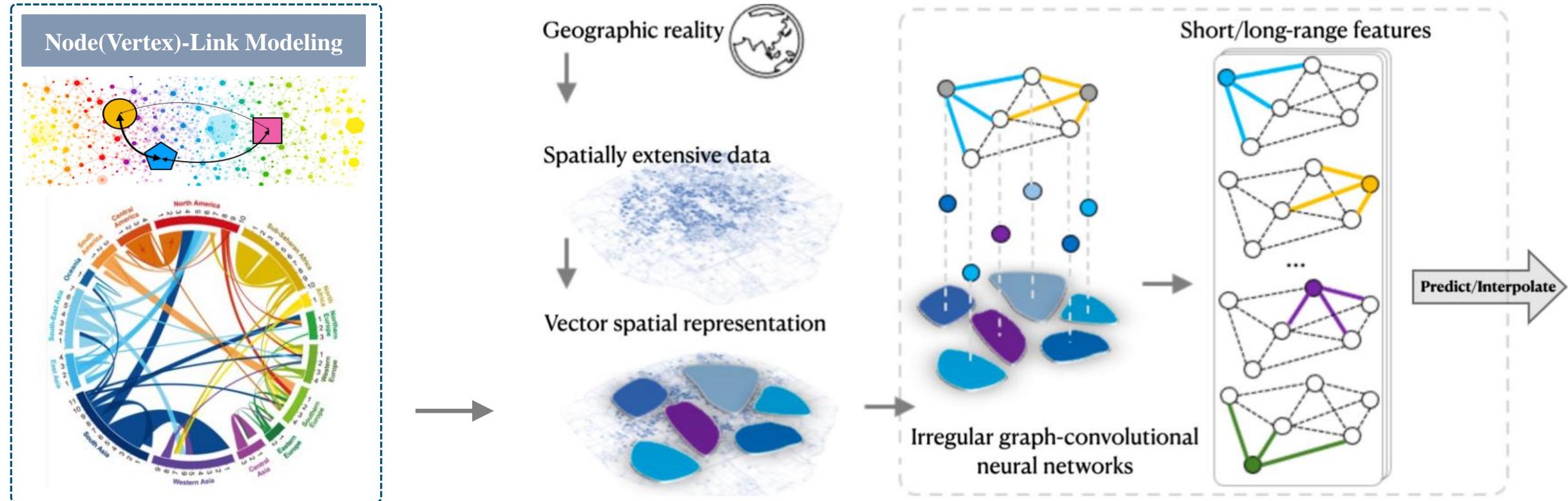


There Is Significant Divergence On Points After Poverty Line Using Representation Learning

# Representation Learning On Graph

## Graph Representation: How To Make Algorithms Recognize Graph Data?

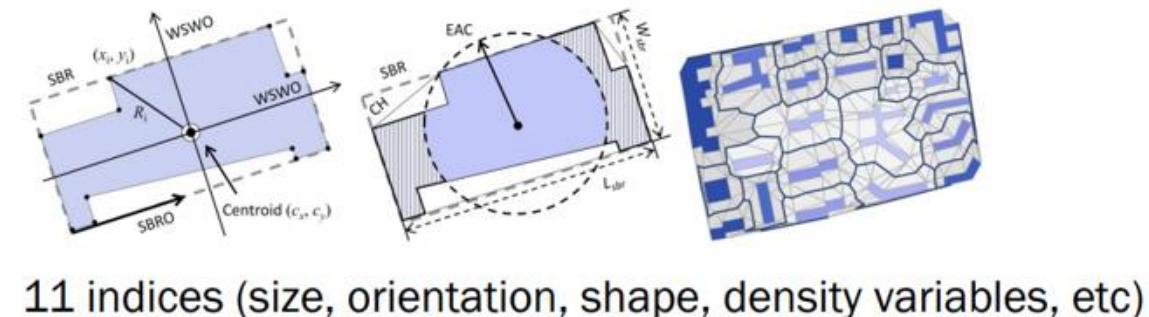
- Utilize GNNs to discover potential interactions within graph data.



# Representation Learning On Graph

## Research Target

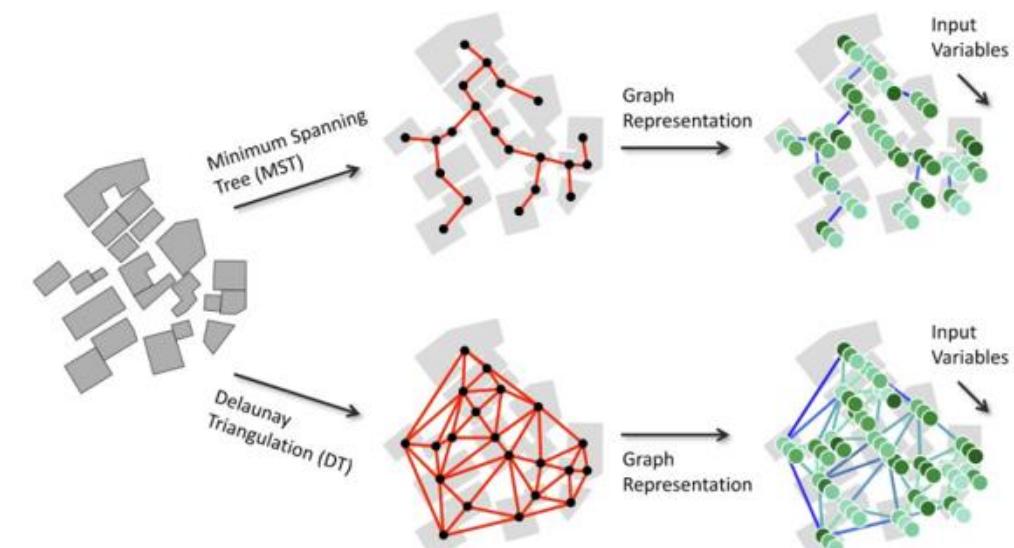
- Building pattern classification using GNNs;
- Model spatial vector data as graph.



11 indices (size, orientation, shape, density variables, etc)

## Methodology

- Graph representations for building groups
  - Each individual building as **vertex** of network;
  - Using 11 indices to summarize the attributes of individual building vertex;
  - The line that connects two buildings' centroids is represented as an edge.



Graph based on DT or MST

Graph representation for a building group constructed with DT and MST (Yan et.al, 2020)

## Heterogeneity-Aware Deep Learning In GeoAI

### □ How to make algorithms understand spatial heterogeneity?

- Spatial problems are difficult to described by a single model with a single set of parameters;
- Spatial coordinates should not be naively added as input features to machine/deep learning algorithms, which may otherwise lead to **overfitting** and **limit model generalizability**.

### □ Categories Of Heterogeneity-Aware Deep Learning

- Performance Driven
- Fairness Driven

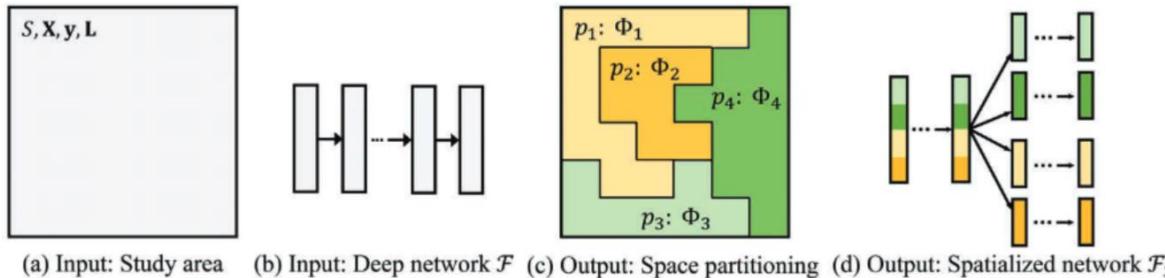


The Spatial Distribution Of Birds  
从直觉上来讲，林地与裸地的鸟类分布有所差异，不能用同一套参数进行建模。

# Heterogeneity-Aware Deep Learning

## Performance Driven

- **Target** : focus on the overall prediction quality;
- **Results** : Spatial-partitioning. Each spatial partition belongs to the same data generation process by parameter  $\theta$ .



Framework Of Performance Driven

## Fairness Driven

- **Target**: reduce the variation of prediction quality.
- **Results**: Model parameter  $\theta$ . It is the same for data samples at all locations.

Accuracy	Spatially Fair			Spatially Biased			
	80%			80%			
Global	80%	80%	80%	Sub-regions	100%	100%	100%
	80%	80%	80%	80%	40%	100%	100%
	80%	80%	80%	100%	40%	40%	40%

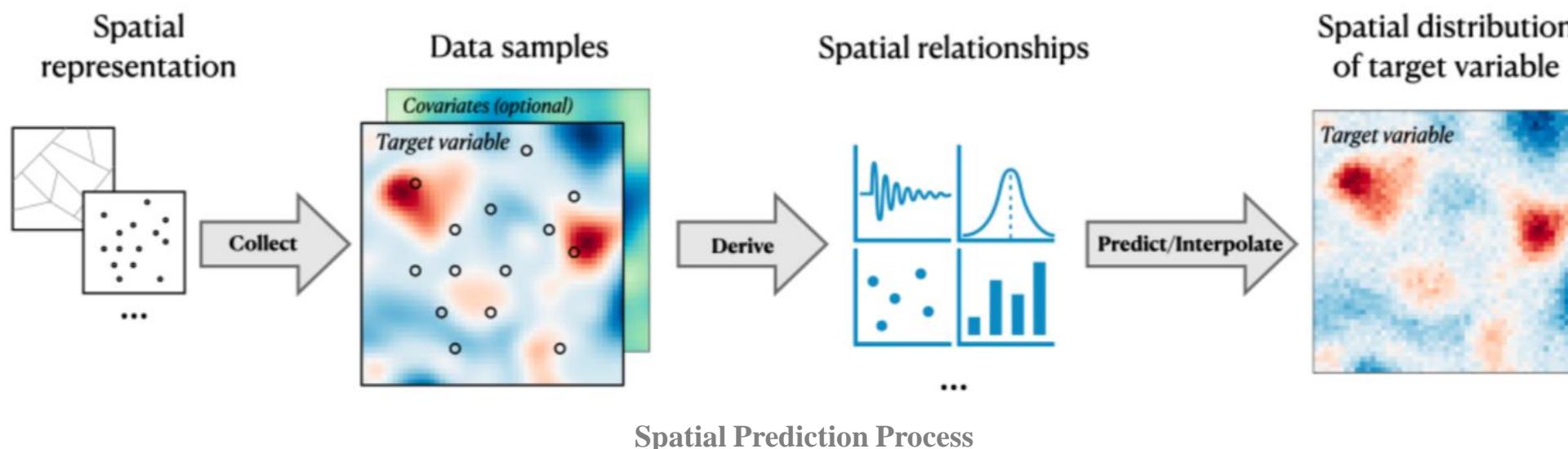
Framework Of Fairness Driven

# Model And Prediction In GeoAI

## Model And Prediction In GeoAI

**Basic Topic:** predict the values of the variable at unobserved location based on sample data.

- First, a set of **sampling locations** are selected over the area of interest;
- Second, the spatial structure of these sampling locations is defined, then data samples collected at these locations are analyzed to derive the **spatial relationships**.
- Finally, these derived relationships are used to **predict** the values of the target variable.

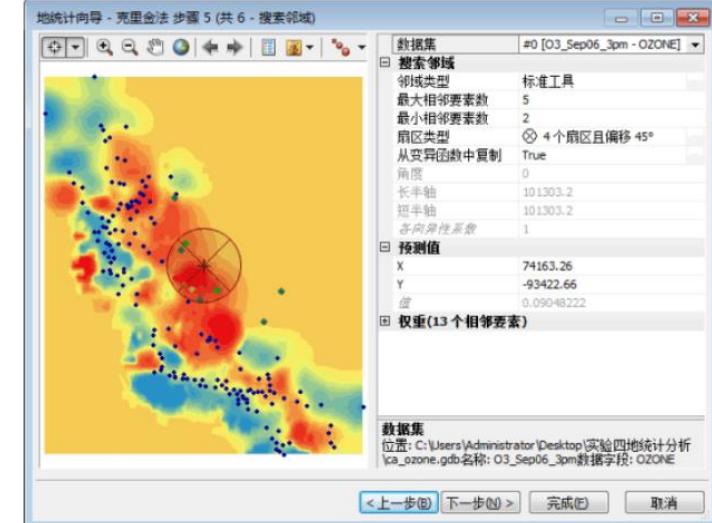
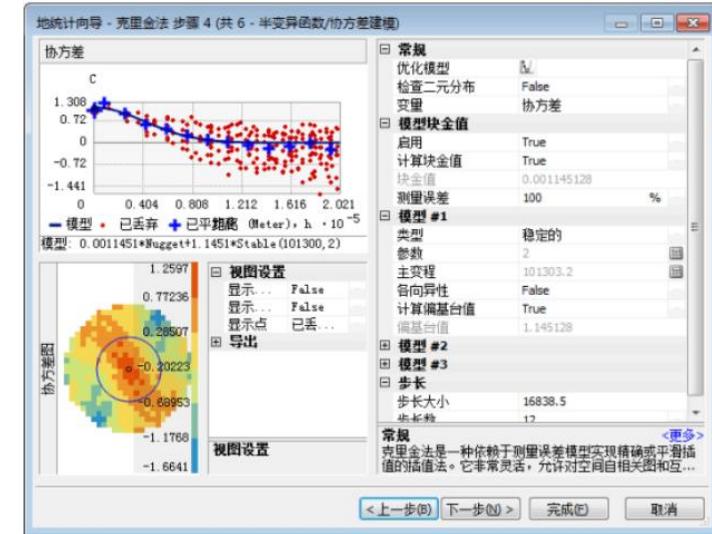


## Geographic phenomena Modeling And Prediction In GeoAI

- The key to the success and applicability of spatial prediction lies in the **basic assumptions used to describe spatial relationships** and the **way these relationships are characterized** in the model. **Most existing methods** follow classical statistical principles, prior domain knowledge, and classical computational paradigms, while **the nature of spatial dependence and heterogeneity** is much more complex than classical statistical models.
  
- **Solution :** Incorporate machine learning and deep learning into **Geostatistics** and **Spatial Regression**, and clarify the impact of these integrations on spatial prediction and geographic knowledge discovery.

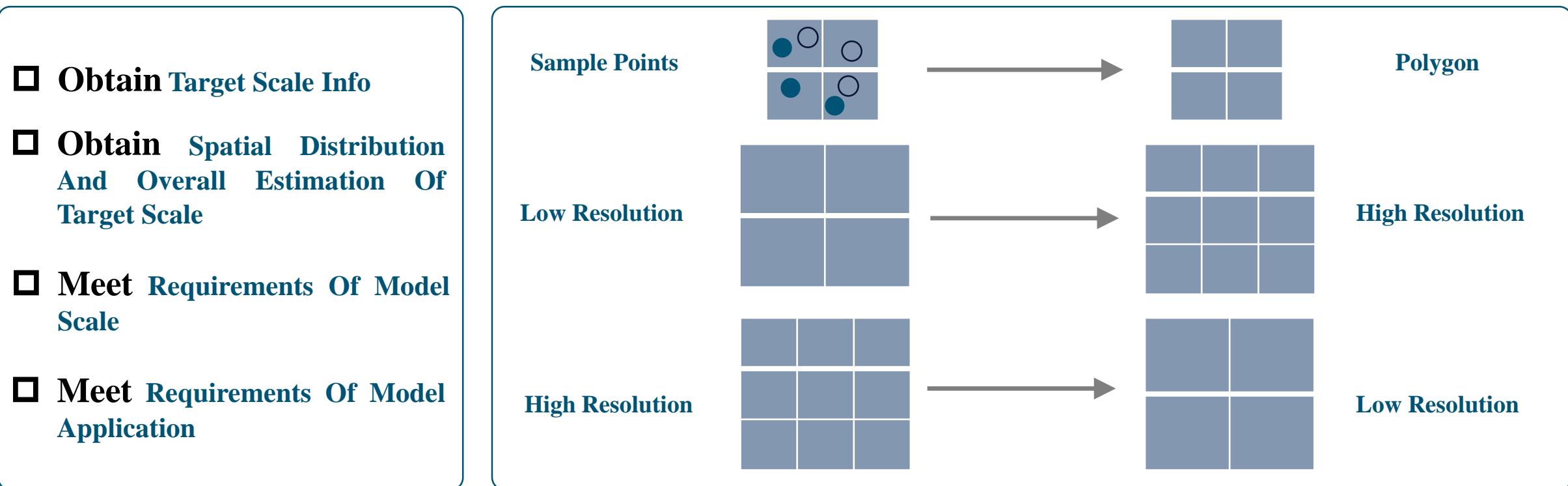
## Geostatistics

- A class of statistics used to analyze and predict the values associated with spatial or spatiotemporal phenomena.
- Geostatistics are quite effective in modeling spatial dependency and quantifying uncertainty in spatial estimation.
  - Geostatistics assume spatial variations can be modeled using simple distance functions, and that spatial patterns are fixed throughout the entire study area.
  - These assumptions make these methods perform well in situations where the **study area is homogeneous**.
  - The corresponding methods perform poor where the **study area is complex and spatially heterogeneous**.



## Case Study Of Geostatistics: Scale Conversion Of Spatial Data

- Target: Obtain target scale information through scale conversion to meet the requirements of the model and application



## Research Target

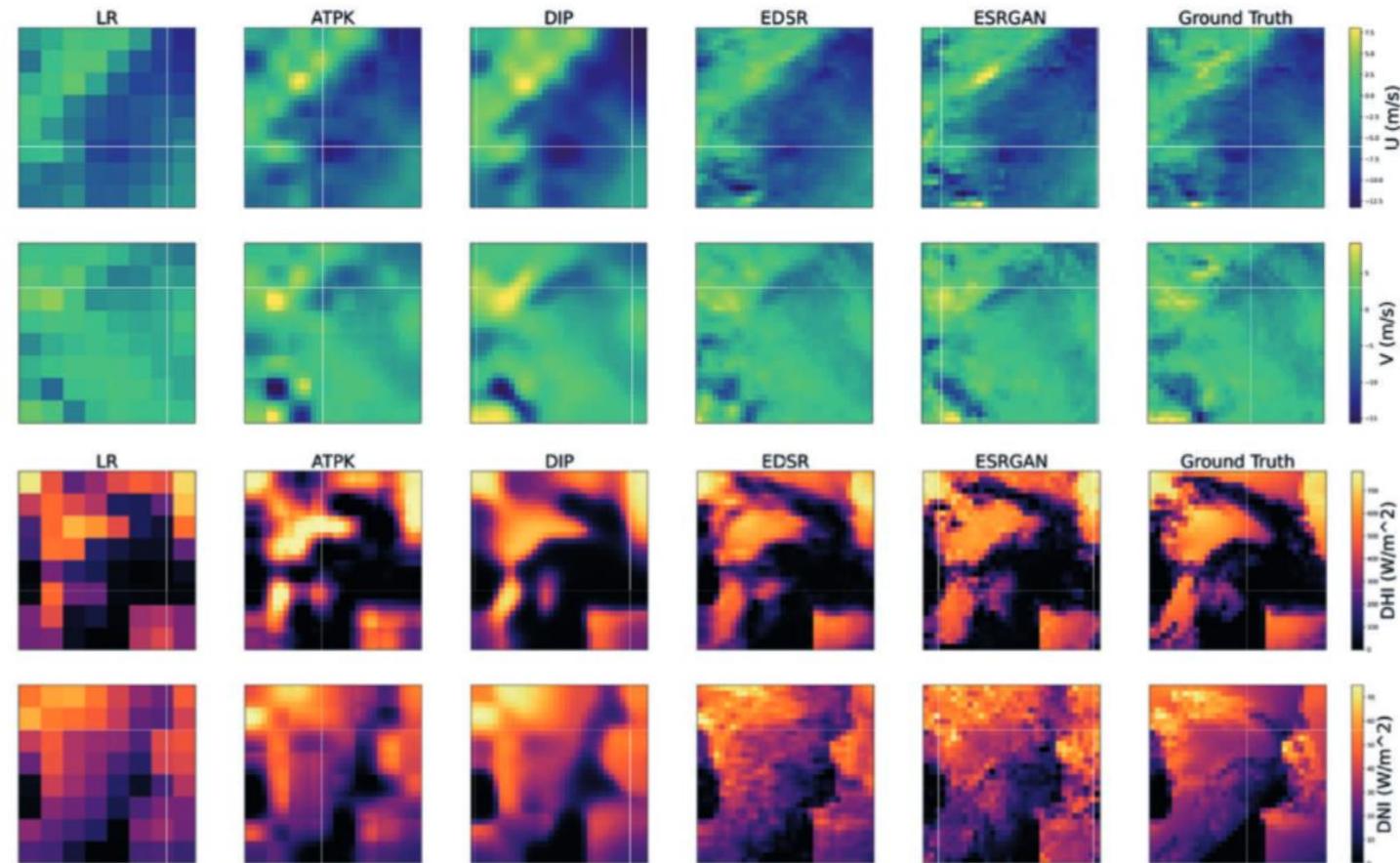
- Compare accuracy performance of traditional Kriging and DL on scale downscaling task.

## Data

- Wind and solar raster data.

## Conclusion

- Deep learning models significantly enhance image quality by discerning spatial distribution within data.



Wind (top) And Solar (bottom) Raster Generated By Different Models. On The Far Left Is The Data To Be Scaled, On The Far Right Is The Actual Data, And The Other are results generated by different model.

## Spatial Regression

- **Spatial regression:** predict development of spatial phenomena based on its spatiality.
- **Classical patterns of spatial econometrics:**
  1. **Employ a spatial adjacent matrix to depict spatial dependence of geographic phenomena.**
  2. **Specification.**
    - Spatial Autoregressive (**SAR**) ; Spatial Error Model (**SEM**) ;
    - Spatial Durbin Model (**SDM**) ; Geographically Weighted Regression (**GWR**) ;
  3. **Identification.**
    - Ordinary Least Square (**OLS**) ; Maximum Likelihood Estimation (**MLE**) ;
    - Instrumental Variables (**IV**) ; Generalized Method of Moments (**GMM**) ;
  4. **Make predictions using identified model.**

## Limitations Of Classical Statistical Analysis

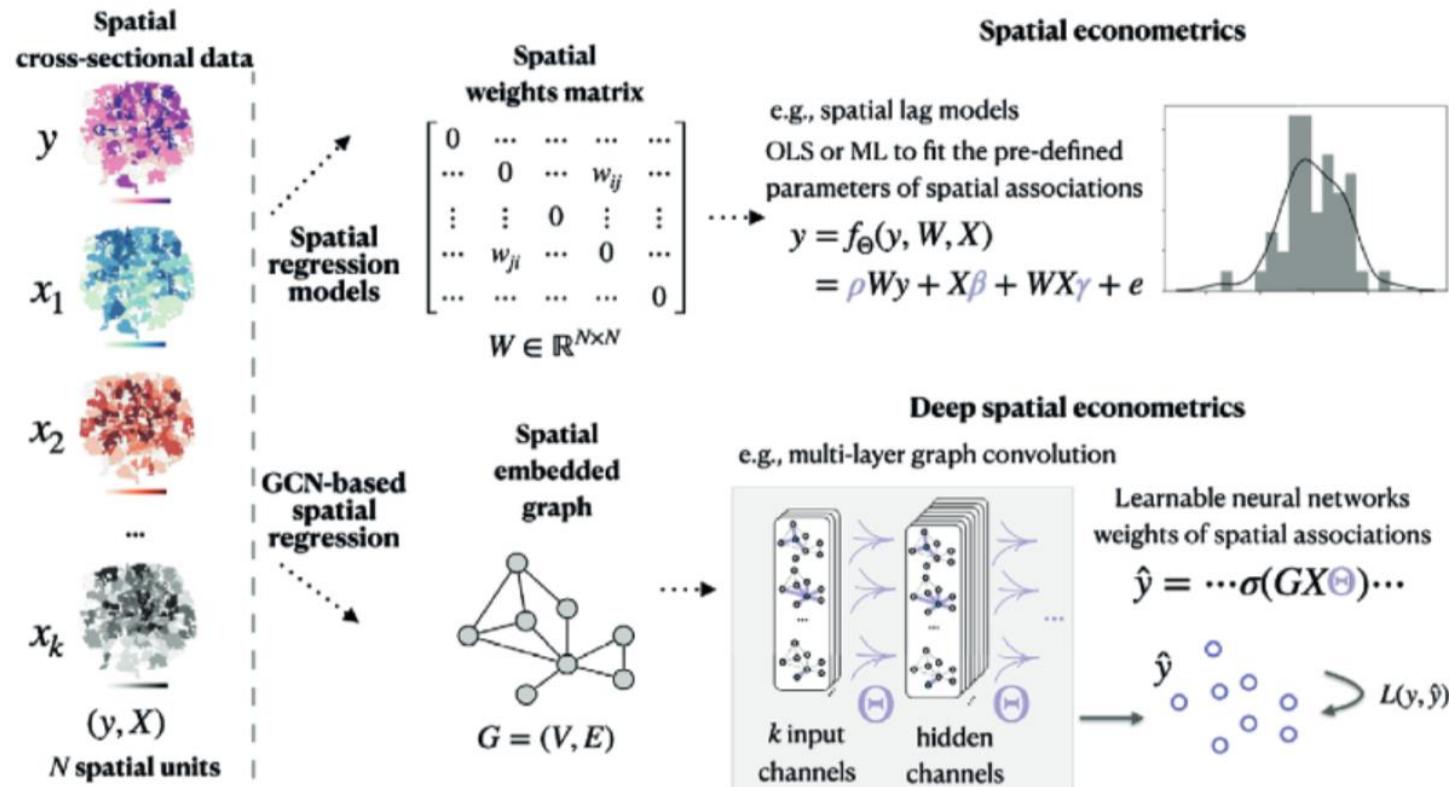
- Classical statistical analysis neglect the non-linear nature of spatial relationships.
- **Gauss-Markov Theory:** How to obtain Best Linear Unbiased Estimations using OLS?
  1. Linear in Parameters;
  2. Random Sampling;
  3. No Perfect Collinearity;
  4. Zero Conditional Mean;
  5. Heteroskedasticity.
- The spatially correlated structures contained in the spatial weight matrix can only be defined between the observed variable positions, without considering other positions of the unobserved variable.
- **The above conditions result in the estimation of spatial relationships being concentrated towards the observed location, which is not an ideal solution for spatial prediction tasks when missing data.**

# Spatial Regression And GeoAI

## AI Methods Addressing Current Issues

- Identify spatial weight matrix using graph convolutional networks(GCN):

- The **feature propagation** mechanism, **spatial locality** nature, and **semi-supervised** training strategy of GCN enable the construction of a conceptual mapping between graph structures and spatial weights.



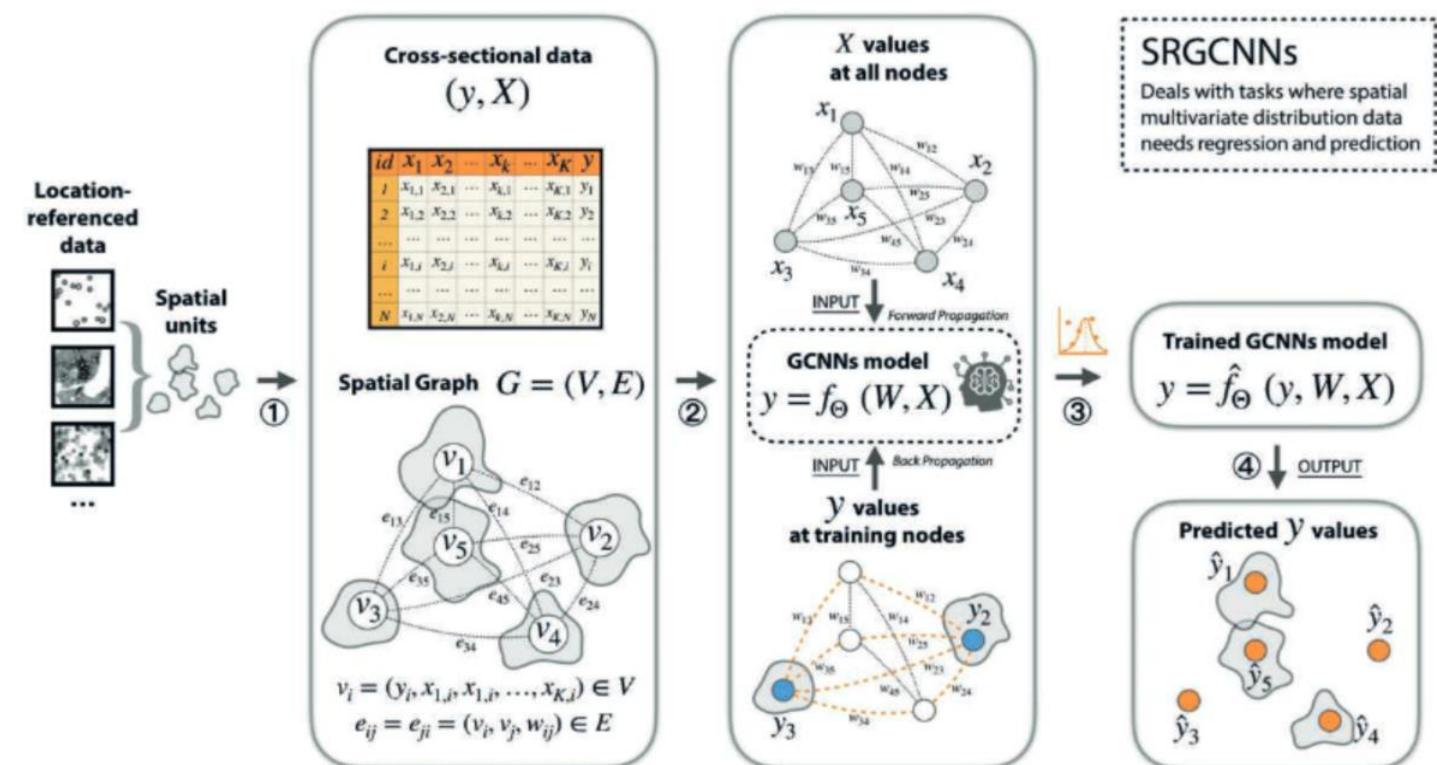
Identify Spatial Weight Matrix using GCN

# Spatial Regression And GeoAI

## AI Methods Addressing Current Issues

- Spatial regression graph convolutional neural networks (SRGCN)

- The similarities between GCN and classical spatial analysis provide insights for researchers to the relationship between **graph convolutional mechanisms** and **fundamental conceptions of spatial regression**.



Comprehensive Workflow For Regression Analysis Of  
Spatial Multivariate Distributions Using SRGCNN

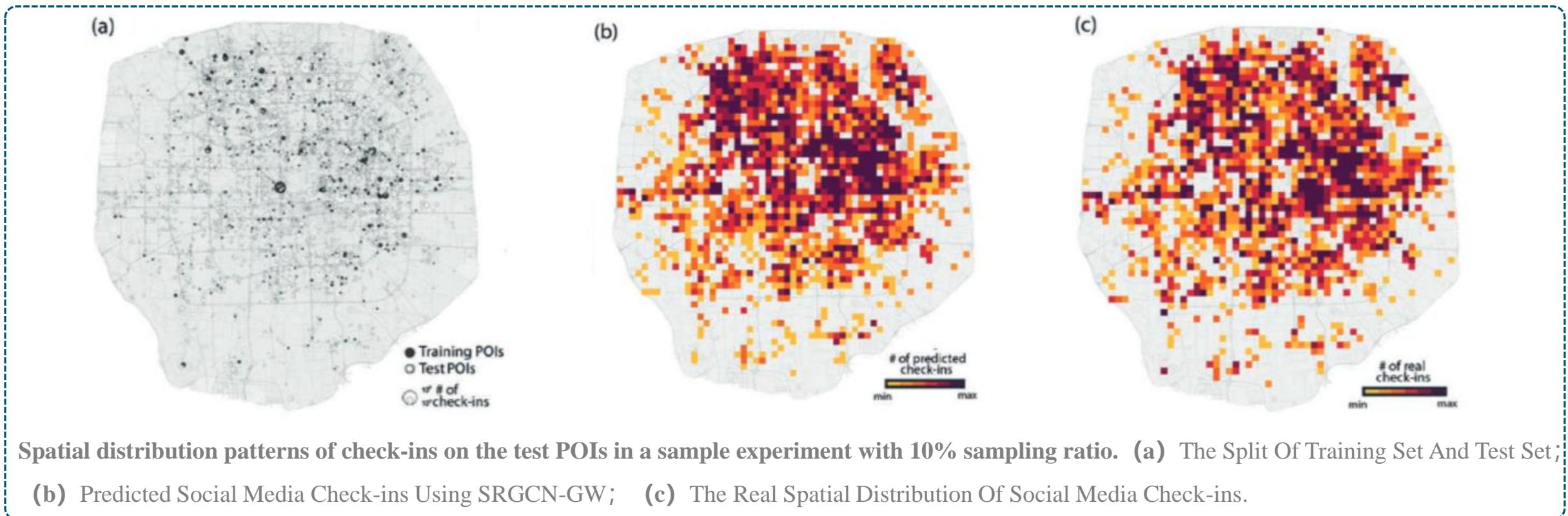
# Spatial Regression And GeoAI

## Research Target

- Predict social media check-ins in Beijing on the POIs.

## Methodology

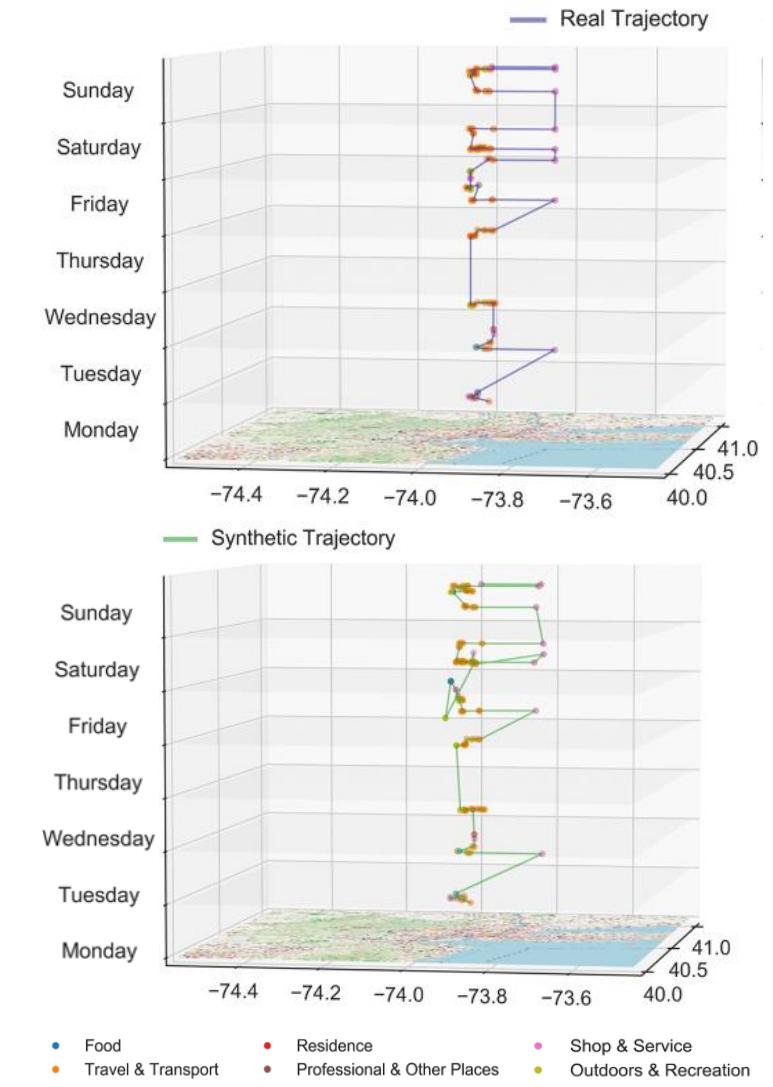
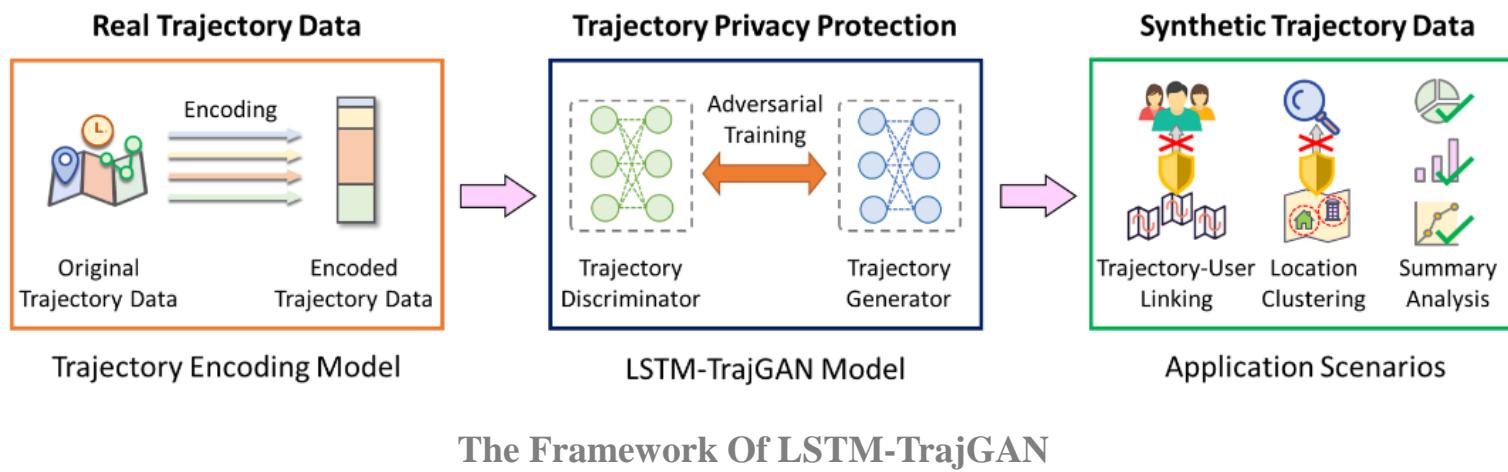
- SRGCN**;
- SRGCN-GW**: An integration of GWR and SRGCN.



# Simulation

## The Application Of GeoAI In Simulation: Case 1

- An end-to-end model to generate privacy preserving synthetic trajectory data for data sharing and publication;
- The black box ensures the **efficiency of private protection**;
- Measure the **spatio-temporal similarities** between synthetic and real trajectories using **original TrajLoss**.



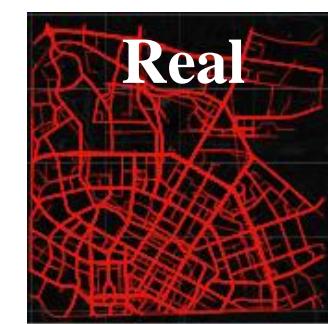
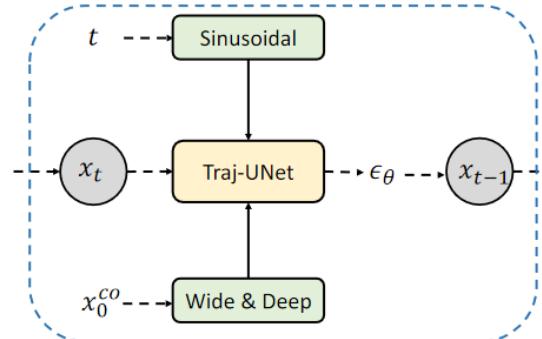
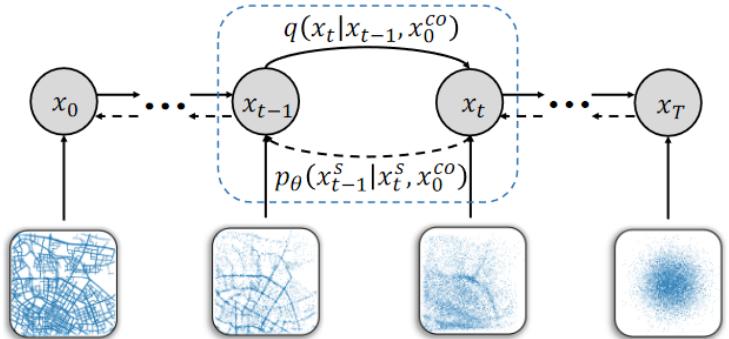
## The Application Of GeoAI In Simulation: Case 2

**Research Target:** Spatial-temporal diffusion probabilistic model for trajectory generation.

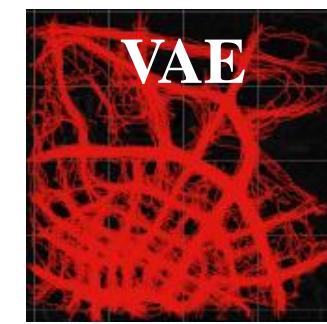
- Combine the generative abilities of diffusion models with the features derived from real trajectories.;

**Research Intuition:**

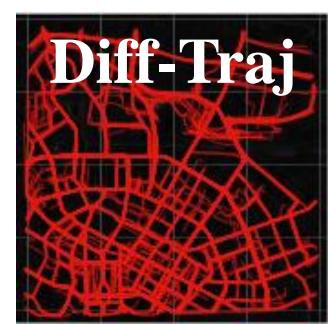
- Synthesize geographic trajectories from white noise through a **reverse trajectory denoising process**, which is in line with the stochastic and uncertain characteristics of human behaviors.



Real



VAE

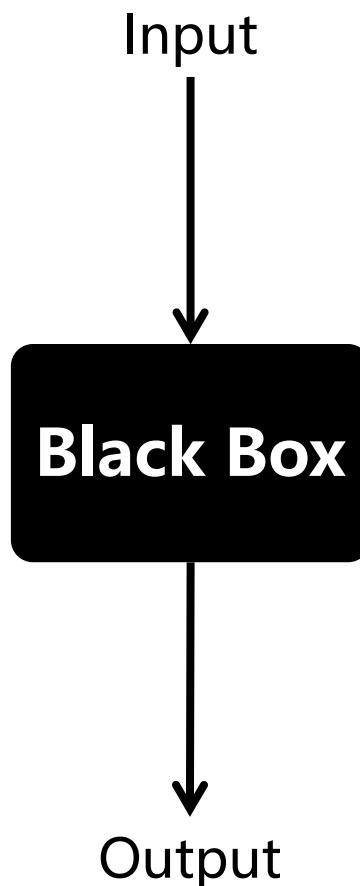


Diff-Traj

The Comprehensive Trajectory Simulation Framework Using Diffusion Model

# Explainability Of GeoAI

**AI is a black box:** it is hard to understand the basis of machine decision-making.

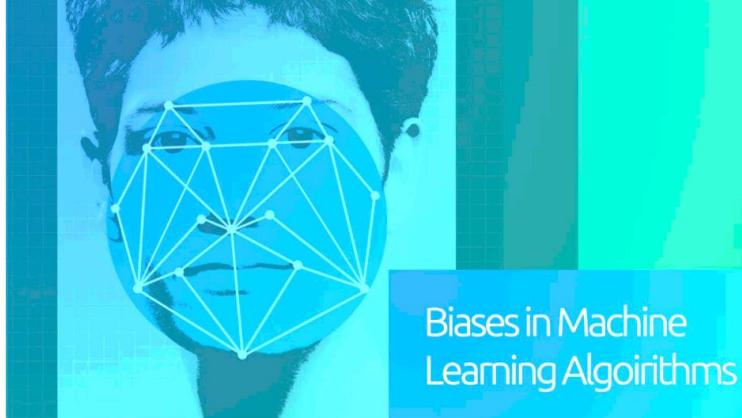


**Carnegie Mellon University**

 Machine Learning Department | Carnegie Mellon University School of Computer Science

About      Academics      Research      People      Honors and Awards

> News > News Archive > 2016-2020 > 2018 > october > Amazon Scraps Secret AI Recruiting Engine that Showed Biases Against Women



October 11, 2018  
Amazon Scraps Secret AI Recruiting Engine that Showed Biases Against Women  
AI Research scientists at Amazon uncovered biases against women on their recruiting machine learning engine  
By Roberto Iriondo

Potential Gender Discrimination In AI Algorithms



Misunderstanding Of Prompts

# Explainability Of GeoAI

## How to reveal what AI algorithms have actually learned?

- Spatial Explicit Artificial Intelligence: integration of AI algorithms and prior knowledge;
- Explainable AI(XAI)



# Explainability Of GeoAI

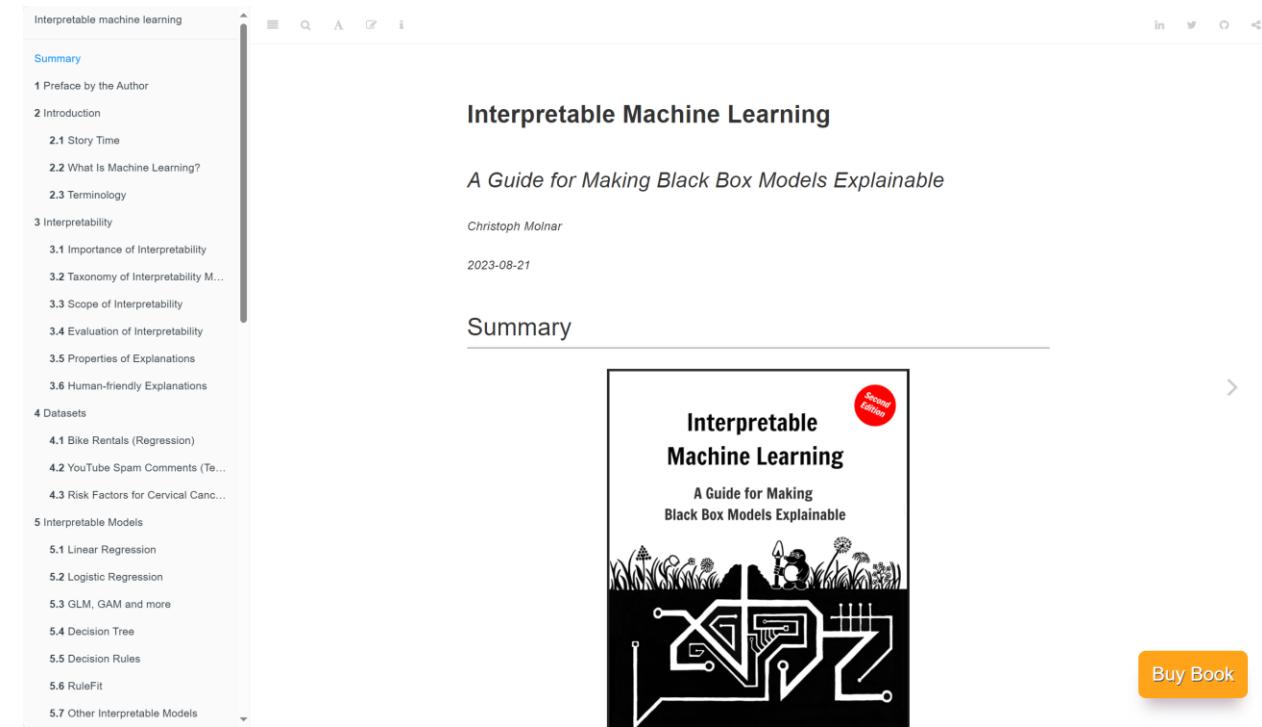
## How to reveal what AI algorithms have actually learned?

- Spatial Explicit Artificial Intelligence: integration of AI algorithms and prior knowledge;
- Explainable AI(XAI)

“**Explainable artificial intelligence (XAI)** is a set of processes and methods that allows human users to comprehend and trust the results and output created by machine learning algorithms.”

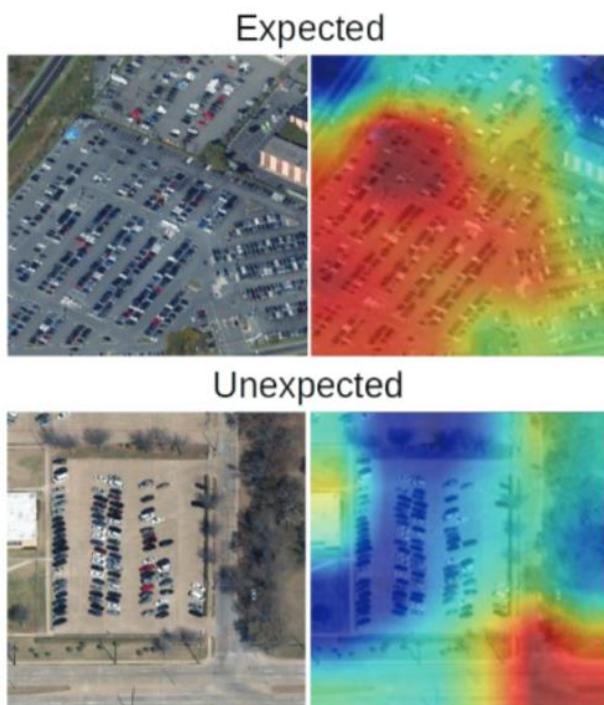
— IBM

Molnar (2020). Interpretable machine learning: a guide for making black box models explainable.  
<https://christophm.github.io/interpretable-ml-book/>



## What Is The Purpose Of Developing XAI?

- Provide insights on model decision process;
- Explore the unknown.



### □ Research Target:

Classify parking lot based on remote sensing images.

### □ Methodology

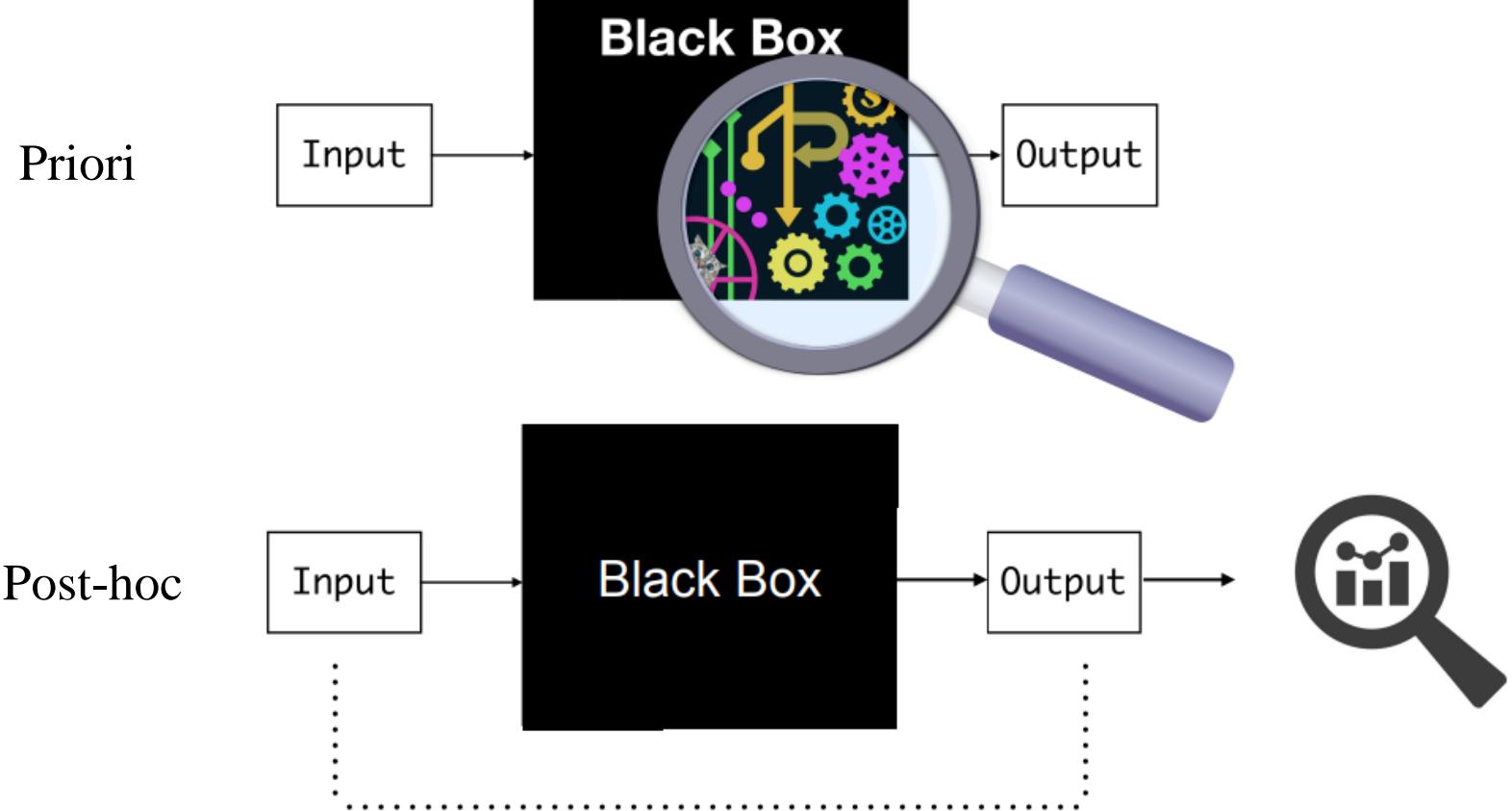
Explore the principles of model decision using XAI. A warm color denotes an important pixel that contributes to the corresponding task.

### □ Conclusion

Many vehicles are **expected** to be the key feature, however, the **use of other features** such as the way to the parking lot is **unexpected**.

## Types Of XAI

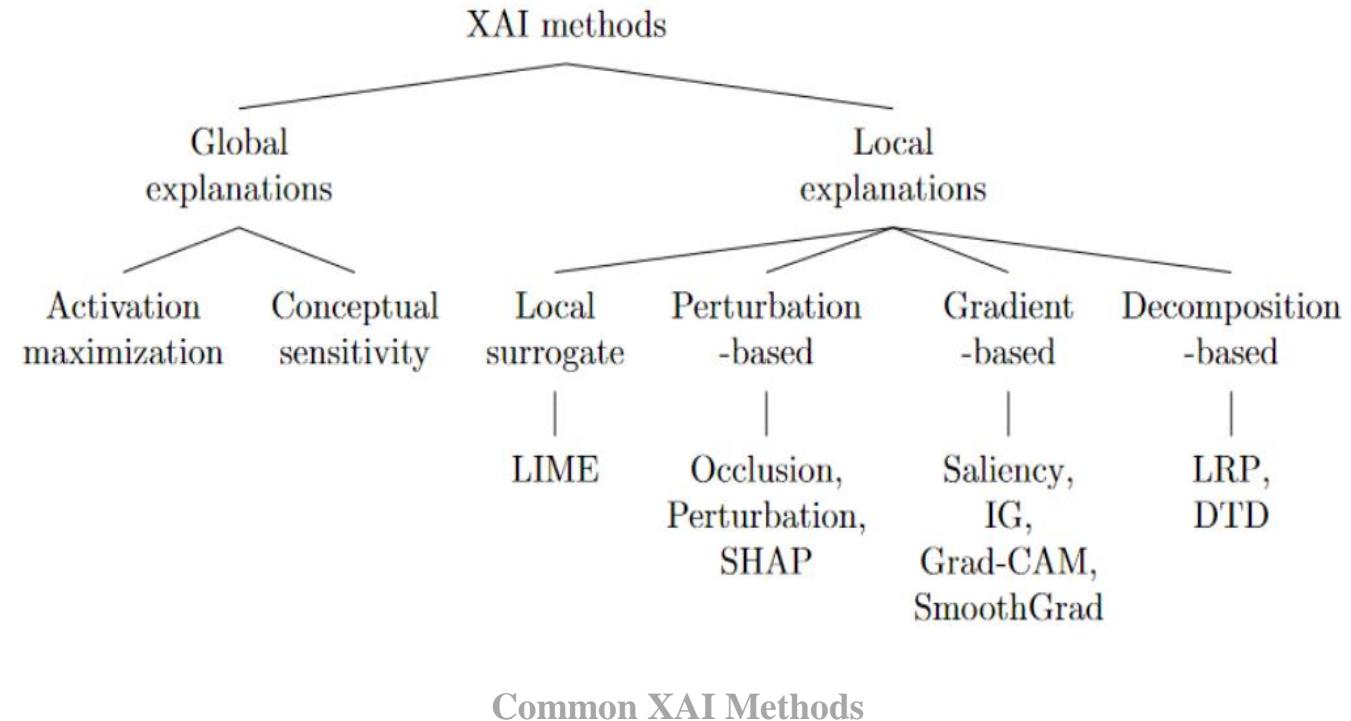
- Priori (Model-Based);
- Post-hoc (Model Free).



Realization Of Two Types Of XAI (Murdoch et al., 2019)

## Global & Local Interpretation

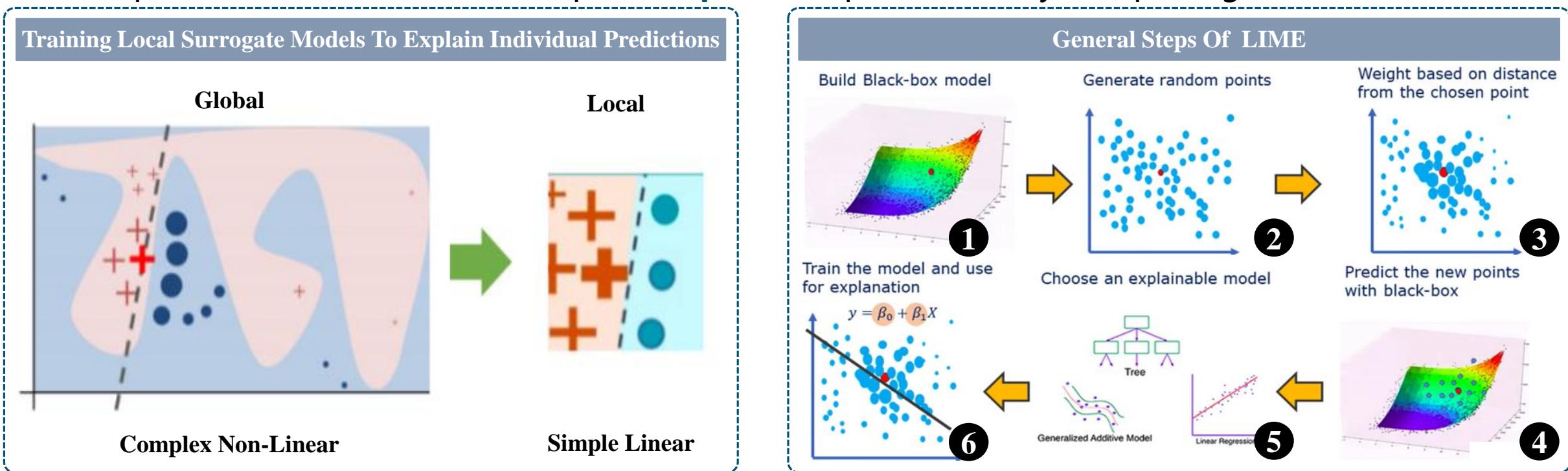
- **Global** : The interpretation of all samples (predictions).
  - E.g. Global importance of features.
- **Local**: The interpretation of individual predictions.
  - E.g. Local dependency.



In the following section, we will provide a brief introduction on common XAI methods used in geography and urban science.....

## Local Interpretable Model-agnostic Explanations(LIME)

- Complex non-linear process can be explained using interpretable local models.
- **Sample randomly, Get** black box **predictions** on samples, **Weight** based on distance , **Train** interpretable local models on samples, **Explain** the predictions by interpreting the local model



## Shapley Value

- An explainable methods based on Game Theory in area of machine learning.
- In a game, the average **marginal contribution** of each player to **all possible combinations of possible alliances**.

$$\varphi_i(v) = \frac{\text{Possible permutations}}{\sum_{S \subseteq N \setminus \{i\}} \frac{|S|! (n - |S| - 1)!}{n!} (v(S \cup \{i\}) - v(S))}$$

Marginal contribution



Lloyd Shapley (1923-2016)  
Nobel Prize in Economics (2012)

## Shapley Value

Starting from a simple case: Calculation of **Academic Influence**.

- Assuming we have three authors, each of whom has written articles alone and collaborated. Each article cites as follows:

- |            |                    |
|------------|--------------------|
| • Null: 0  | • {A + B}: 5       |
| • 作者A: 5   | • {A + C}: 120     |
| • 作者B: 10  | • {B + C}: 140     |
| • 作者C: 100 | • {A + B + C}: 150 |

- What is the academic influence of each article based on their citations and author combinations?

# Shapley Value, SHAP

	A Marginal Contributions	B Marginal Contributions	C Marginal Contributions	Probs	Total
ABC	5	(A+B) - A	(A+B+C) - (A+B)	1/6	150
ACB	5	(A+B+C) - (A+C)	(A+C)-A	1/6	150
BAC	(A+B)-B	10	(A+B+C) - (A+B)	1/6	150
BCA	(A+B+C) - (A+B)	10	(B+C) - B	1/6	150
CAB	(A+C) - C	(A+B+C) - (A+C)	100	1/6	150
CBA	(A+B+C) - (B+C)	(B+C) - C	100	1/6	150

	A Marginal Contributions	B Marginal Contributions	C Marginal Contributions	Probs	Total
ABC	5	0	145	1/6	150
ACB	5	30	115	1/6	150
BAC	-5	10	145	1/6	150
BCA	10	10	130	1/6	150
CAB	20	30	100	1/6	150
CBA	10	40	100	1/6	150
Shapley Value	7.5	20	122.5	1	150

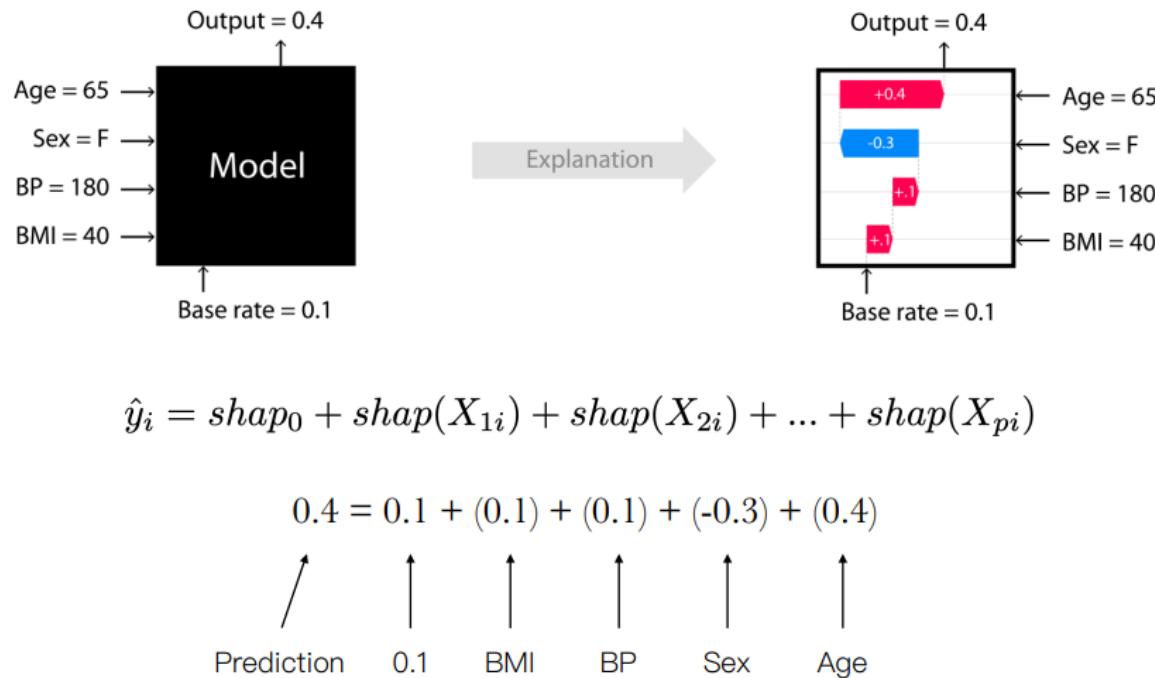
- The method of calculating the academic influence using Shapley values is shown in the upper left table, and the calculation results are shown in the upper right table;
- In practical scenarios, it is impossible to measure the contribution of each element and explain the black box model by manually calculating Shapley values (NP-Hard);
- **SHAP provides a series of effective methods to estimate Shapley value.**
- **The site of SHAP python package:** <https://github.com/slundberg/shap>.

Lundberg & Lee. (2017). A unified approach to interpreting model predictions. Advances in neural information processing systems, 30.

Lundberg, et al. (2020). From local explanations to global understanding with explainable AI for trees. Nature machine intelligence, 2(1), 56-67.

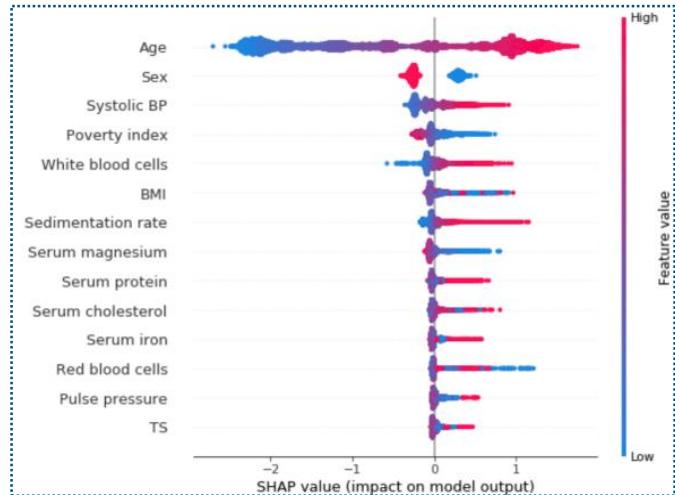
## SHAP

- Engineering solutions for explaining machine learning models;
- Integrate by AI platforms of Amazon, Google etc.



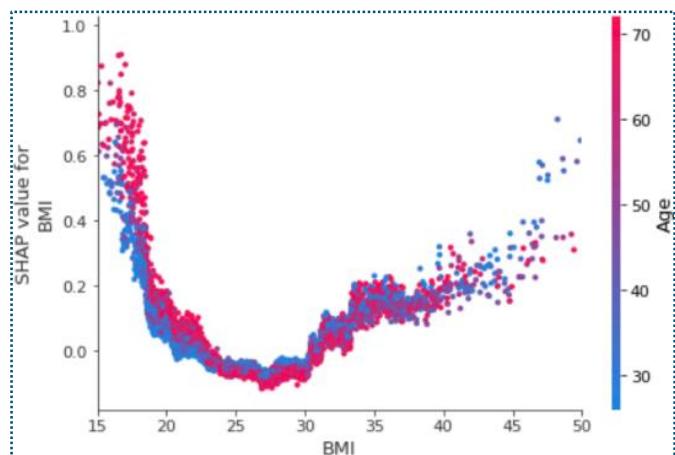
### Feature Importance

- Bee Swarm Plot
- Display the Shapley Values of each individual attributes.



### Local Dependency

- Scatter Plot
- The variation of Shapley value of age when BMI stay unchanged.



## Grad-CAM (Class Activation Mapping)

- Unravel the most important pixels identified by model to interpret the prediction.
- Grad-CAM has a wider range of applications compared to traditional heat map.

### □ Research Target

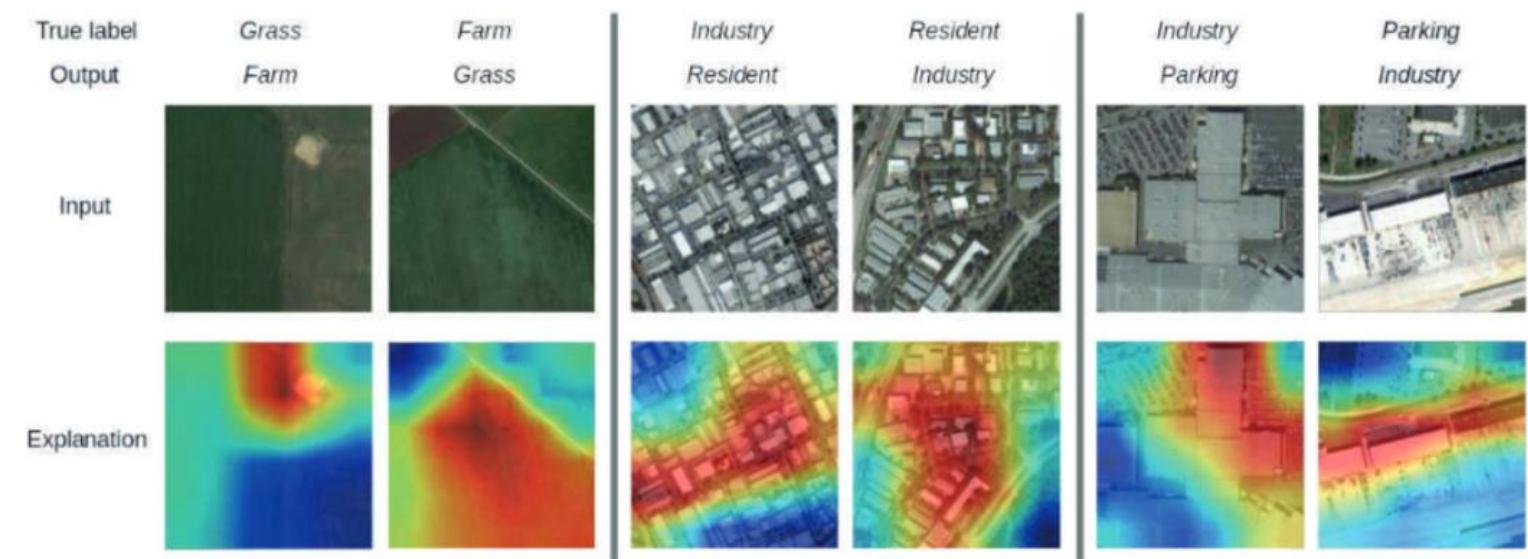
Interpret the results of imagery classification to enhance AI Models

### □ Methodology

Explain confusing samples using XAI.

### □ Conclusion

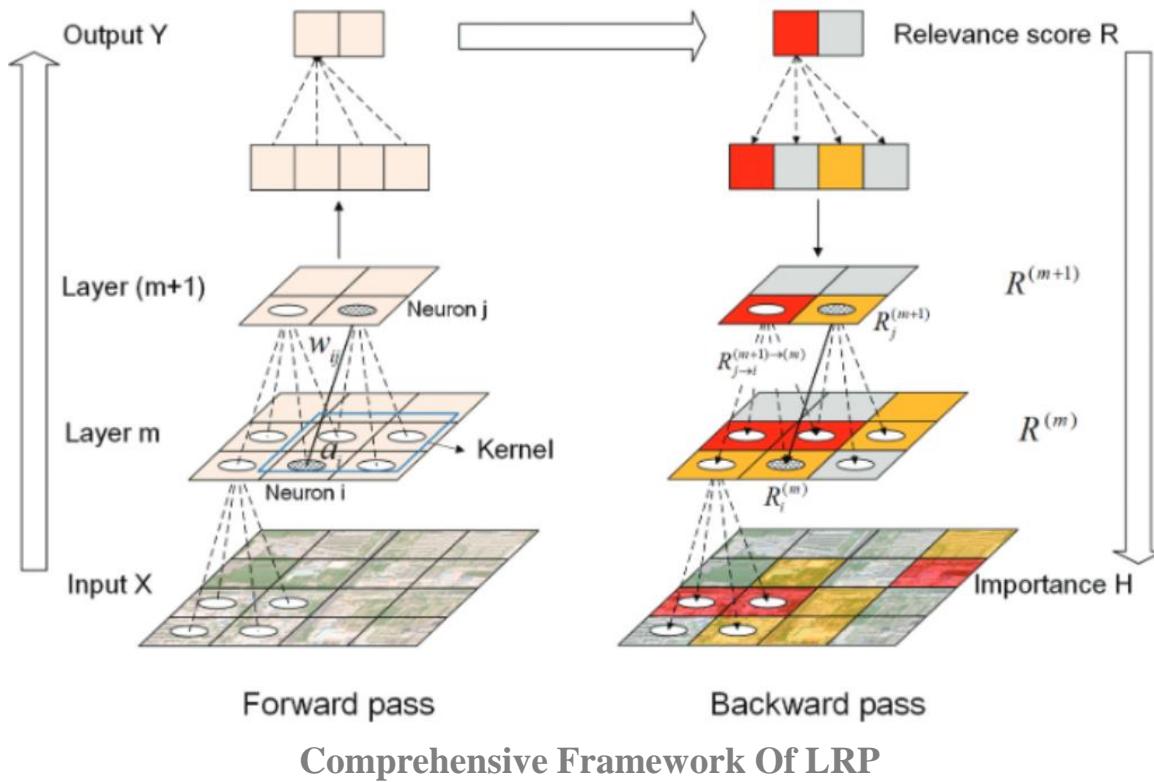
The low accuracy of model can be attribute to the confusion of samples, requiring detailed labeling of data.



Examples Of Wrongly Classified Samples  
A Warm Color Denotes An Important Pixel That Contributes To The Corresponding task

## LRP (Layer-wise Relevance Propagation)

- Extract contribution of each pixel layer by layer.



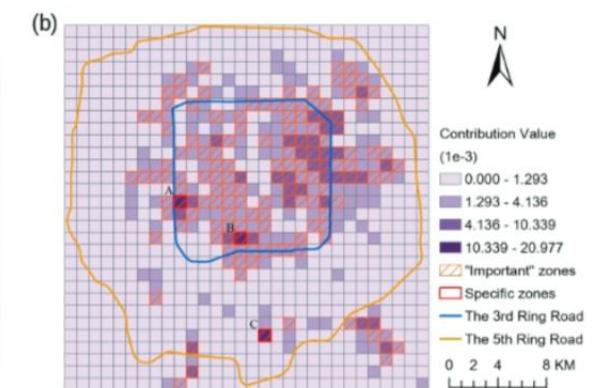
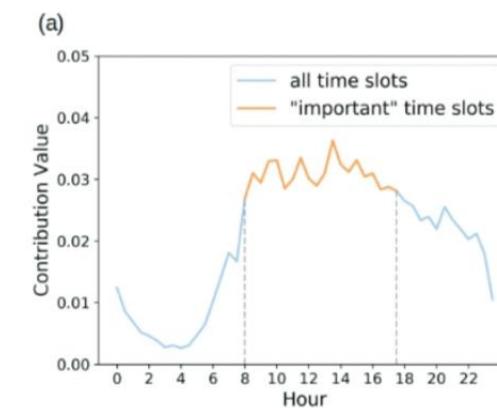
## Case Study Of LRP

### Tar - g e t

Using taxi travel characteristics and DL to predict departure traffic during weekdays and weekends/holidays.

### M e t - h o d s

The units are first sorted by order of contributions, and then the cumulative contribution ratio is calculated. Units that accumulate to over 60% are considered important units.



Bach, S., et al., 2015. On pixel-wise explanations for non-linear classifier decisions by layerwise relevance propagation. PloS ONE, 10 (7), e0130140.

Cheng, X., et al., 2021a. A method to evaluate task-specific importance of spatio-temporal units based on explainable artificial intelligence. International Journal of Geographical Information Science, 35 (10), 2002–2025

## Another Black Box: The Interpretation Of XAI

- The accuracy of interpretation is important for understanding the real behaviors of model.
- **Open XAI is necessary for industry practice.**



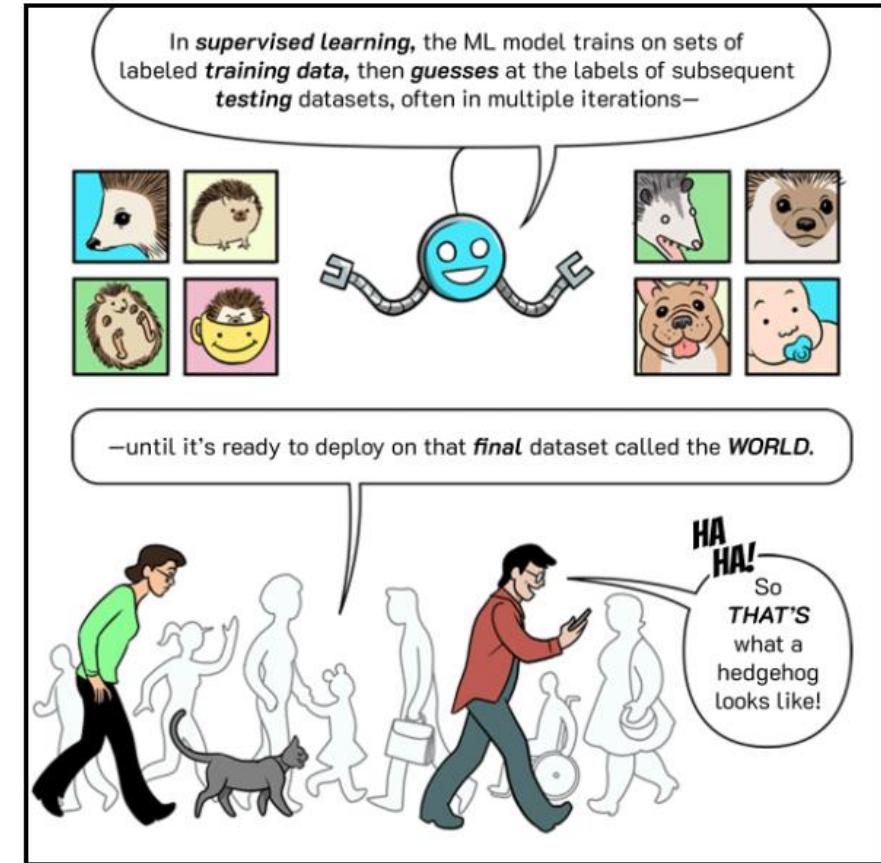
## Challenges for Engineers: Explaining Models with Large Parameters

- The calculation of Shapley Values is expensive, consuming both computing power and time.
- **Solutions:**
  - Reduce the dimension of features;
  - Design more effective algorithms.....

# Generalization Of GeoAI

## Evaluate Generalization Ability Of Model

- Split samples into training set, test set and validation set by employing **cross validation** (CV).
- In general, data scientists fit model on training set and test set, and assess ability of **model generalization** on validation test.
- Traditional method of cross validation is not appropriate to deal with **spatial data with heterogeneity**.
- **Spatial Cross Validation (SCV)** partitions sample data sample data based on their spatial distribution instead of random allocation, addressing potential biases introduced by spatiality.

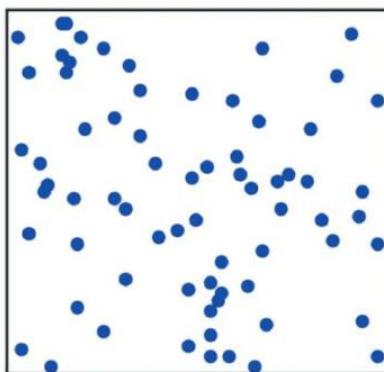


Generalization refers to the ability of a trained model to perform well on unseen inputs during training, making AI applications reliable to cope with the diversity of real-world scenarios

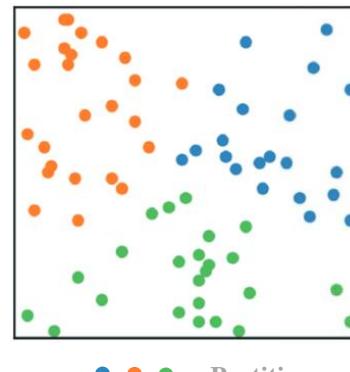
# Spatial Cross Validation

## Main Spatial CV Methods

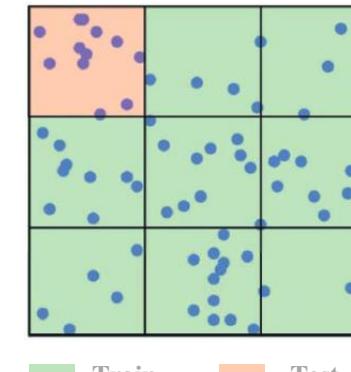
- **Cluster-based SCV:** Partition samples based on their coordinate and clustering algorithms;
- **Grid-based SCV:** Divide research area into grid cells, and partition data basis on these grids;
- **Geo-attribute-based SCV:** Split data based on spatial regions defined by geo-attribute;
- **Spatial leave-one-out CV:** Extension of tradition leave-one-out. Create a buffer zone surrounding the validation data. Data falling into the buffer zone will not be used for model training.



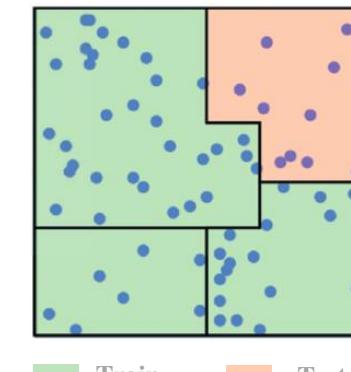
Original Data



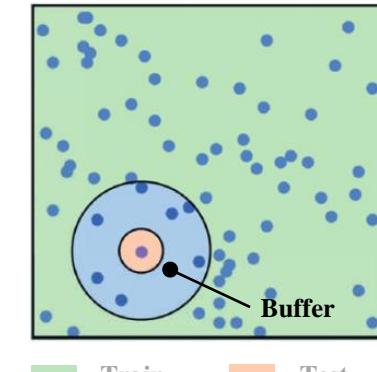
Cluster-based



Grid-based



Geo-attribute-based



Spatial leave-one-out

# Spatial Cross Validation

## □ Research Target

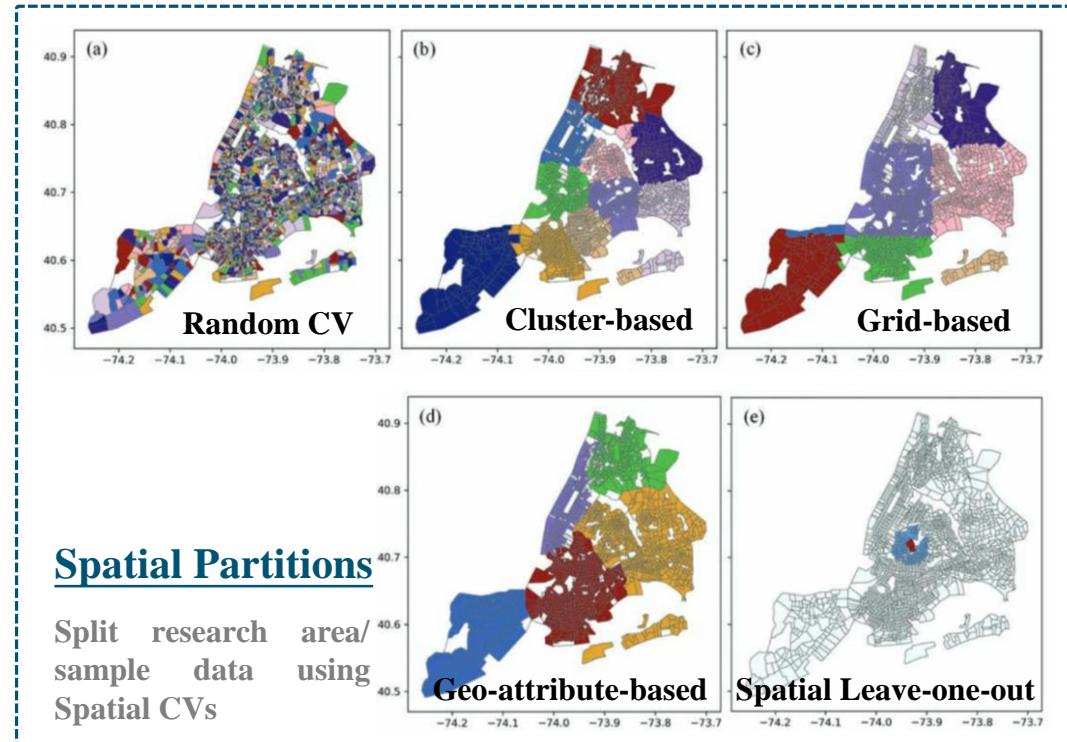
Predict the obesity rate in New York using DL.

## □ Methodology

Employ Spatial CV we mentioned above to assess the accuracy of models, and compare the results with random allocation.

## □ Conclusion

The model's performance on random CV is relatively better than its performance on spatial CVs. Therefore, **using random CV may lead to an overestimation to the model performance**, owing to spatial autocorrelation within data.



## 评估结果

CV method	R2	RMSE
Random CV	0.8692	2.1287
Clustering-based spatial CV	0.7244	3.0899
Grid-based spatial CV	0.7466	2.9624
Geo-attribute-based spatial CV	0.6613	3.4250
Spatial leave-one-out CV	0.8083	2.5766

# The Application Of GeoAI

## GeoAI And Urban System

- Researchers have investigate 581 articles focused on spatially explicit AI published between 2018 and 2022.
- The application of GeoAI in urban systems focuses on the following topic:
  - Social Sensing;
  - Urban Dynamics;
  - Social Differentiation of Urban Areas.

Table 1

List of the reviewed papers. (ANN—Artificial Neural Network; DNN—Deep Neural Network; CNN—Convolutional Neural Network; GNN—Graph Neural Network; CA—Cellular Automata.).

Paper	Methods
<b>Urban Dynamics (urban development)</b>	
He et al. (2018)	CNN+CA
Xu et al. (2019)	ANN+CA
Ou et al. (2019)	Autoencoder+CA
Lu et al. (2020)	ANN+CA
Zhai et al. (2020)	CNN+CA
Rana and Sarkar (2021)	ANN+CA
Gantumur et al. (2022) <sup>a</sup>	ANN+CA
<b>Urban Dynamics (urban population flows)</b>	
Zhang and Cheng (2019)	CNN
Huang (2019)	GNN
Yao et al. (2020)	GNN
Zhang and Cheng (2020)	GNN
Hu et al. (2021)	GNN
Yang et al. (2021)	GNN
Liu et al. (2021b)	GNN
Xia et al. (2021)	GNN
Li et al. (2021a)	GNN
Zhu et al. (2022) <sup>a</sup>	GNN
<b>Social Differentiation of Urban Areas</b>	
Gervasoni et al. (2018)	CNN
De Sabbata and Liu (2019)	Geoconvolution+DNN
Monteiro et al. (2019)	CNN
Zhang et al. (2021)	CNN
<b>Social Sensing</b>	
Zhu et al. (2020b)	GNN
Liu and De Sabbata (2021)	GNN
Zhu et al. (2021)	GNN

<sup>a</sup>Indicates early access.

Liu, P., & Biljecki, F. (2022). A review of spatially-explicit GeoAI applications in Urban Geography. *International Journal of Applied Earth Observation and Geoinformation*, 112, 102936

Casali, Y., Aydin, N. Y., & Comes, T. (2022). Machine learning for spatial analyses in urban areas: a scoping review. *Sustainable Cities and Society*, 85, 104050.

# Spatial Cognition

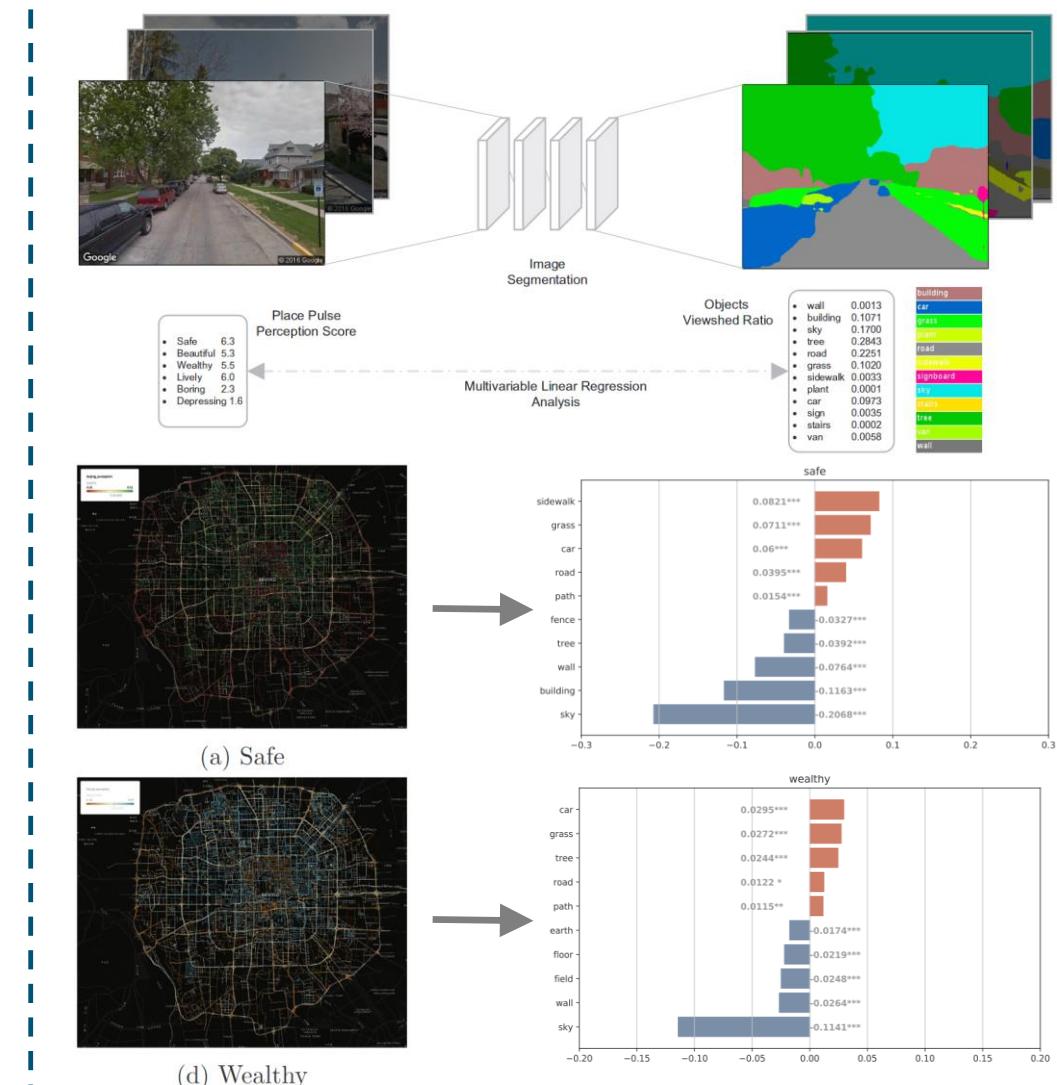
## □ Research Target

Measure human place perceptions, and clarify the relationship between these measurement and the features of the built environment at those place.

## □ Methodology

Propose a data-driven method to measure human perceptions of places in urban areas.

Specifically, train a deep learning model using millions of human ratings of street images. This model is applied to **predict human perception of places** depicted by street view images.



# Spatial Cognition



(a) Safe



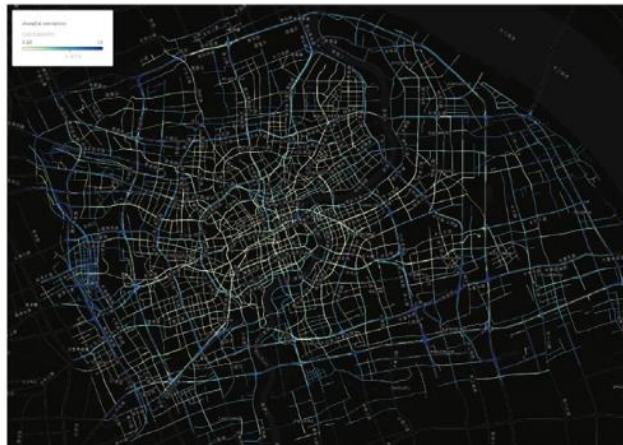
(b) Lively



(c) Beautiful



(d) Wealthy

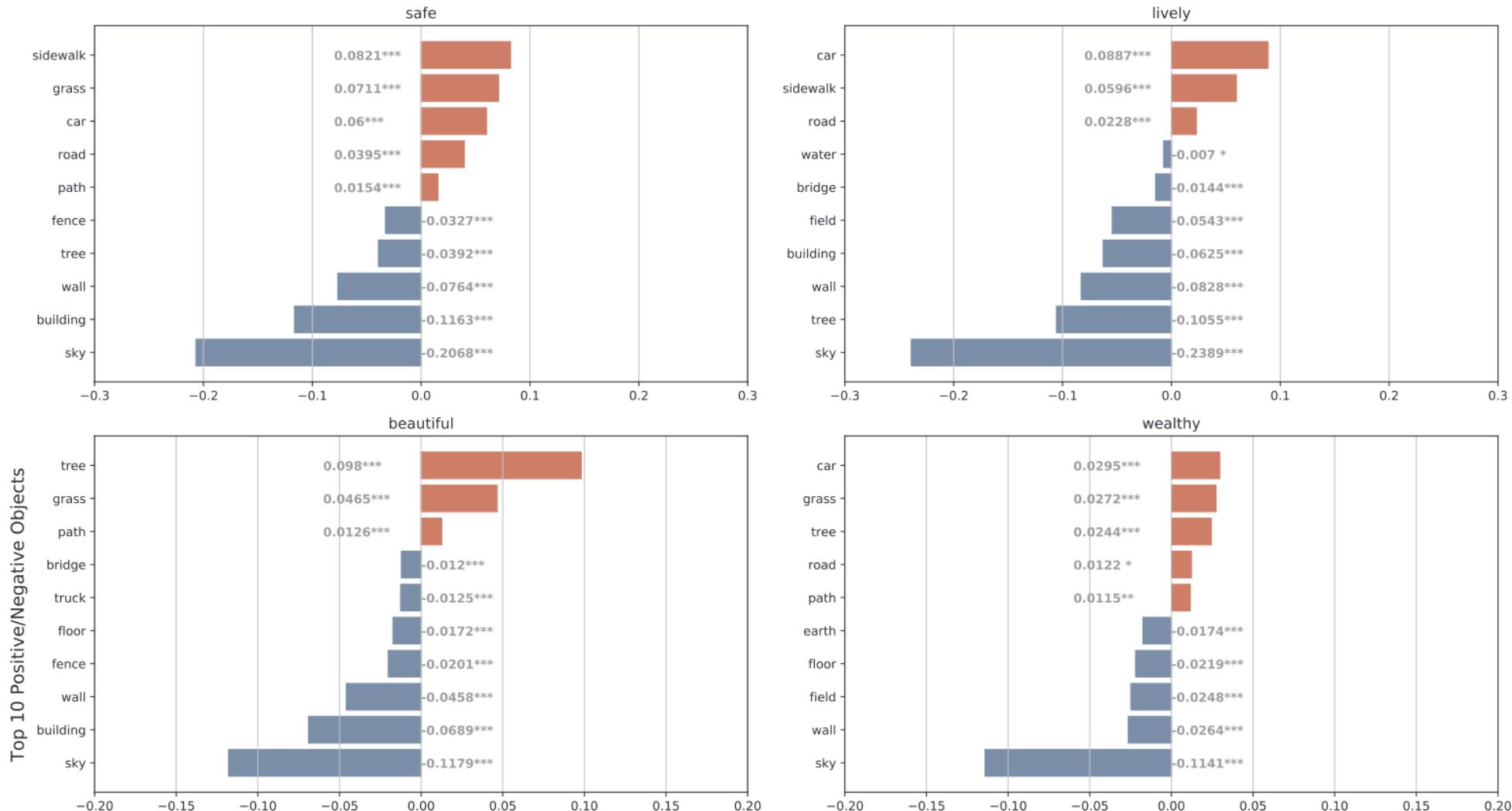


(e) Depressing



(f) Boring

# Spatial Cognition



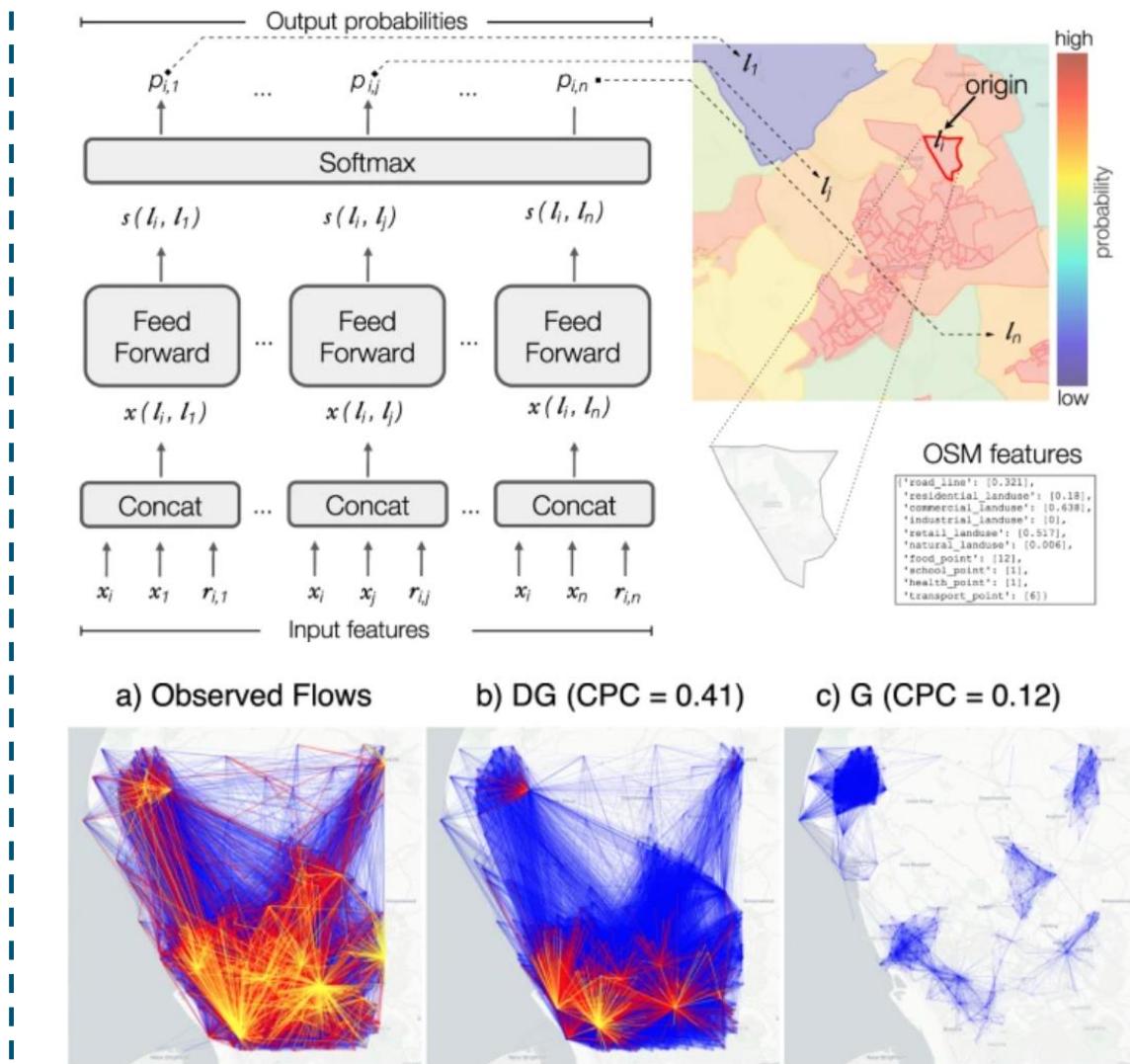
**Model Interpretation:**  
Contributions Of Street  
Visual Elements To  
Human Perceptions.

## Research Target

- Generate flows and predict mobile traffic volumes between two locations by integrating DL and gravity model without historical data.

## Methodology

- Consider the movement between locations as a **classification**.
- **Feature Engineering:** Concatenate attributes of origin and possible destination.
- **Model:** MLP (Not Spatially Explicit) ;
- **Optimization Objective :** CPC divergence between real flow and generated flow.



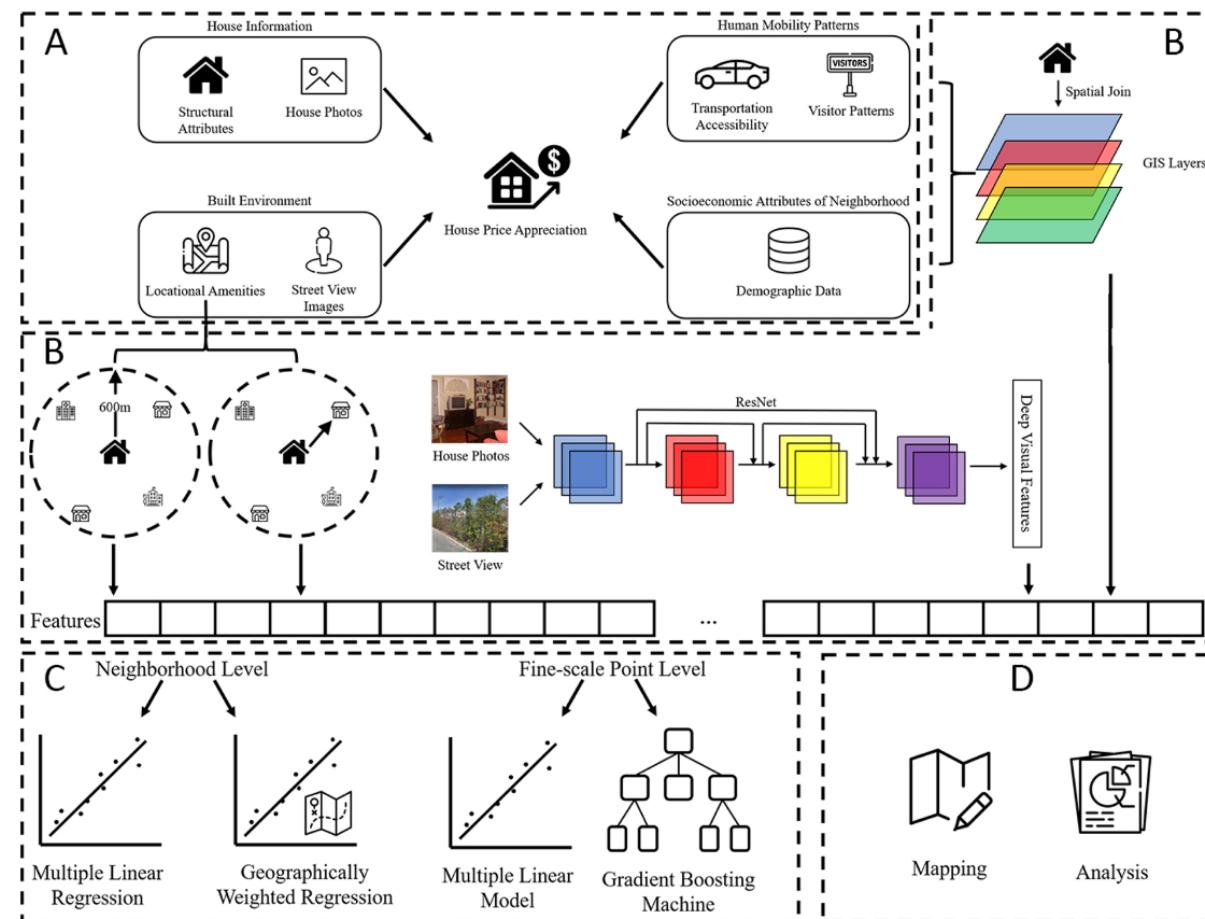
# Social Differentiation of Urban Areas

## Research Target

- Predict house price appreciation using multi-source big geo-data and machine learning.

## Methodology

- **Data Sources** : House information, human mobility patterns, built environment and socioeconomic attributes of neighborhood;
- **Feature Engineer** : Extract features from street view images and house photos;
- **Model**: Machine learning and GWR.

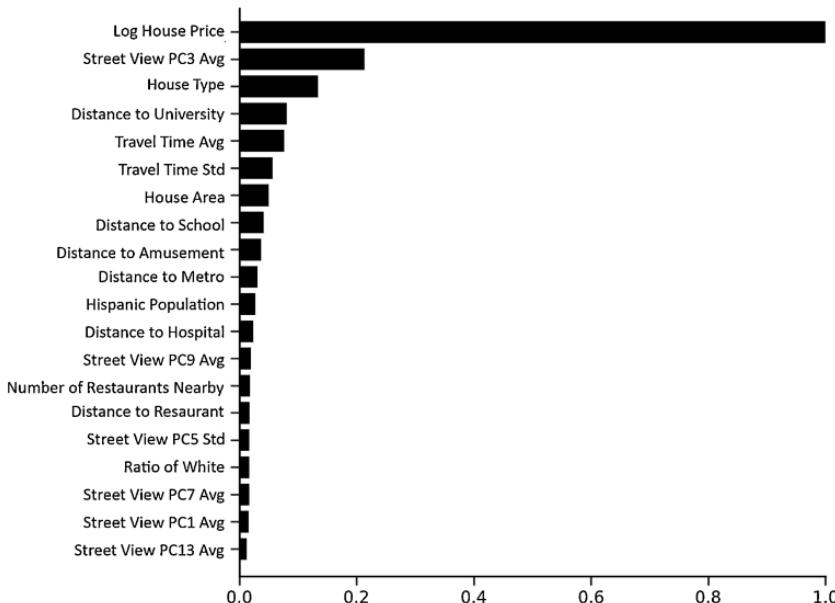


# Social Differentiation of Urban Areas

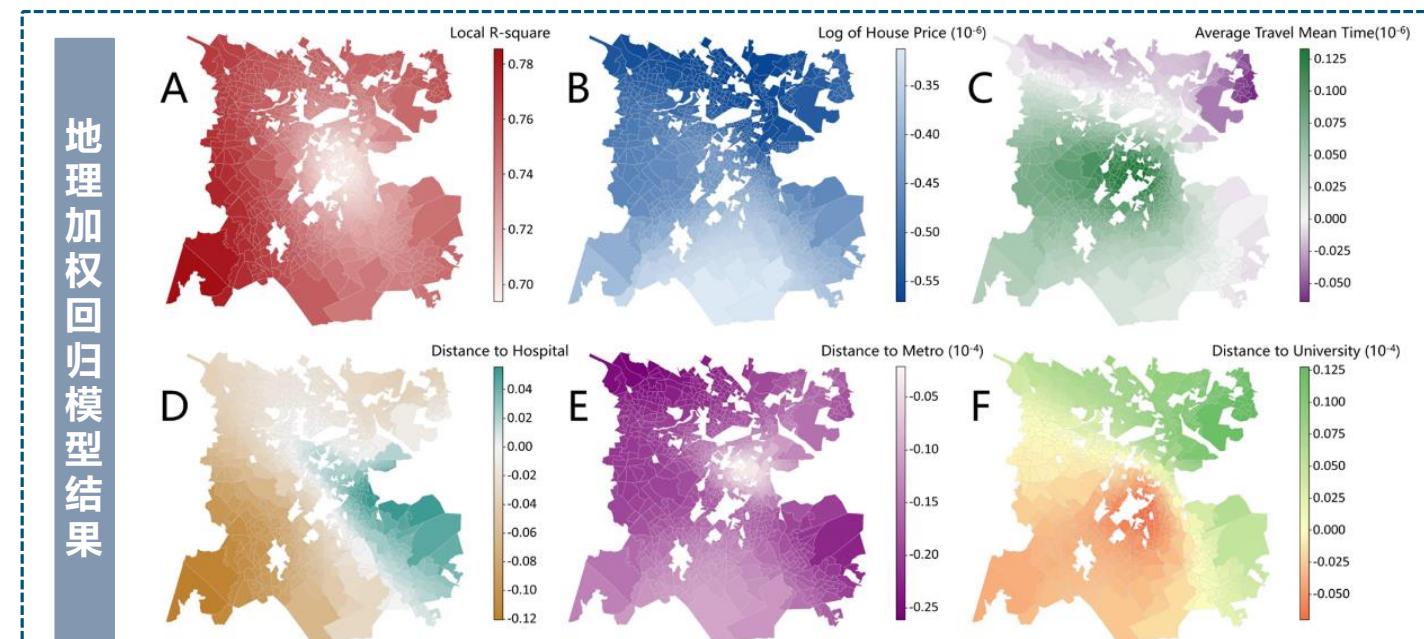
## Conclusion

- GWR provide better prediction and a more holistic explanation for spatial heterogeneity.
- Houses with lower prices and small house area may have higher house appreciation potential.

機器學習模型結果



地理加权回归模型結果



# **Problems And Challenges Of GeoAI**

# Challenges

## □ AI for Social Science **VS** Social Science of AI

### □ Data

- Uncertainty
- Heterogeneity

### □ Scale

- Fairness
- Biases
- Trustworthiness

### □ Mechanism

- Explainability
- Transferability
- Replicability

### □ Application

- Responsibility
- Sustainability
- Privacy

# Thanks

May 28<sup>th</sup>, 2024

1173450209@stu.hit.edu.cn



哈爾濱工業大學(深圳)  
HARBIN INSTITUTE OF TECHNOLOGY, SHENZHEN