北京航空航天大学计算机学院
School of Computer Science and Engineering, Beihang University

KDD2020 San Diego Convention Center San Diego, CA

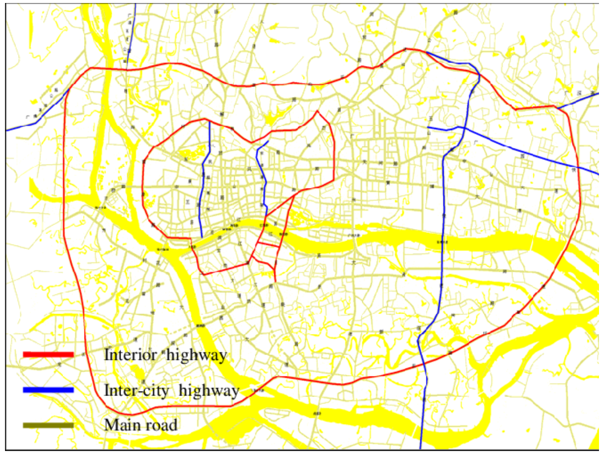
Learning Effective Road Network Representation with Hierarchical Graph Neural Network

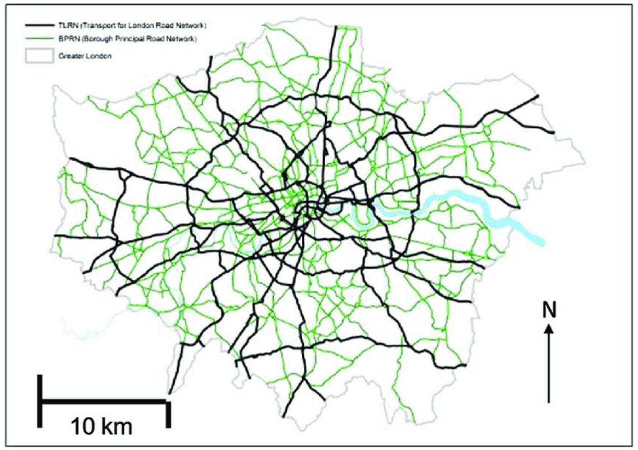
Ning Wu, Wayne Xin Zhao, Jingyuan Wang*, Dayan Pan
School of Computer Science and Engineering, Beihang University
School of Information, Renmin University of China

Background: Personalized Route Recommendation

- Road network is the core component of urban transportation, and it is widely useful in various traffic-related systems and applications.

- It is essential to develop general, effective and robust road network representation models.

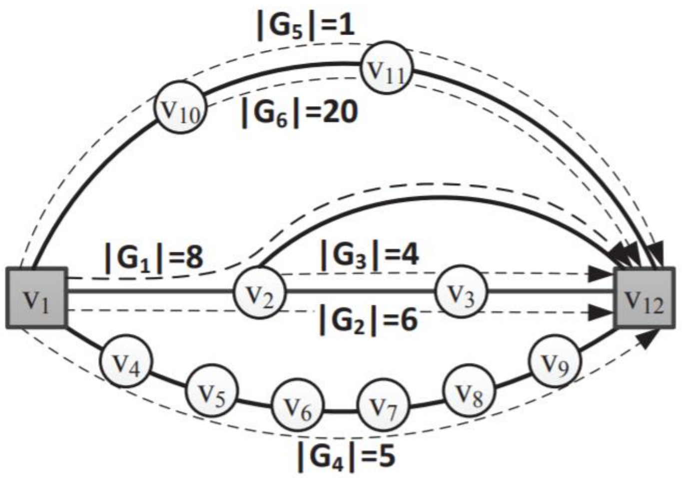




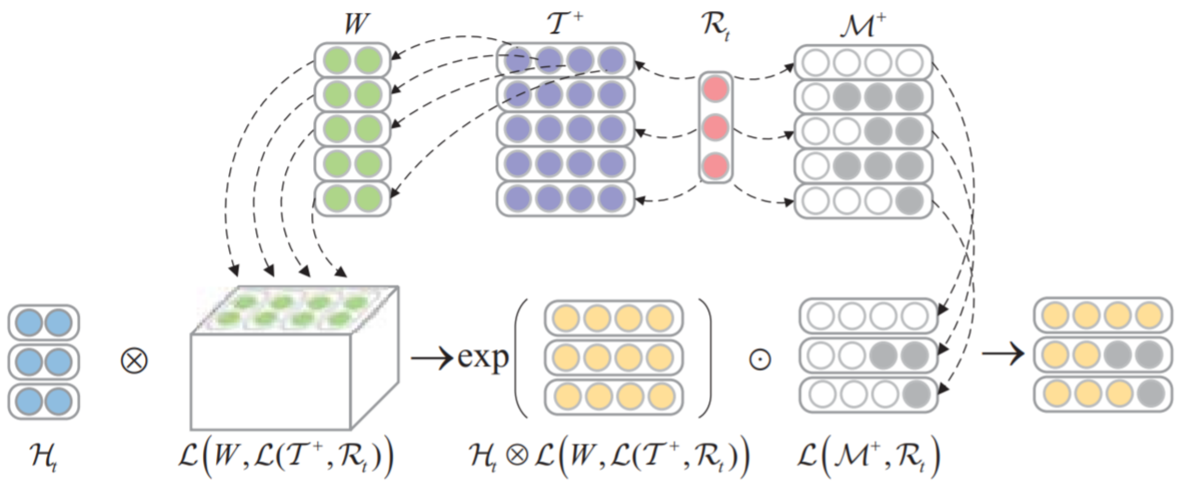
Background: Road Network Modeling

Early Studies:

- Use standard graph algorithm.
- Consider its adjacency matrix as constraint of neural network.



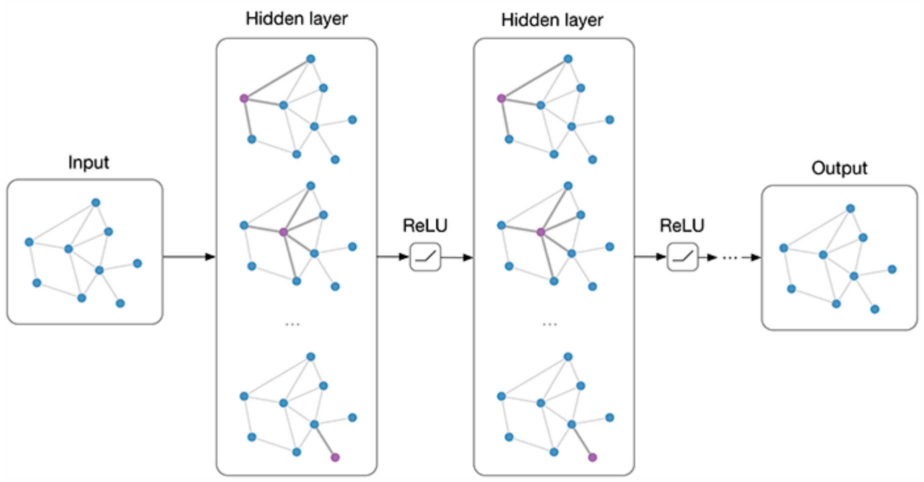
Standard Graph Algorithm

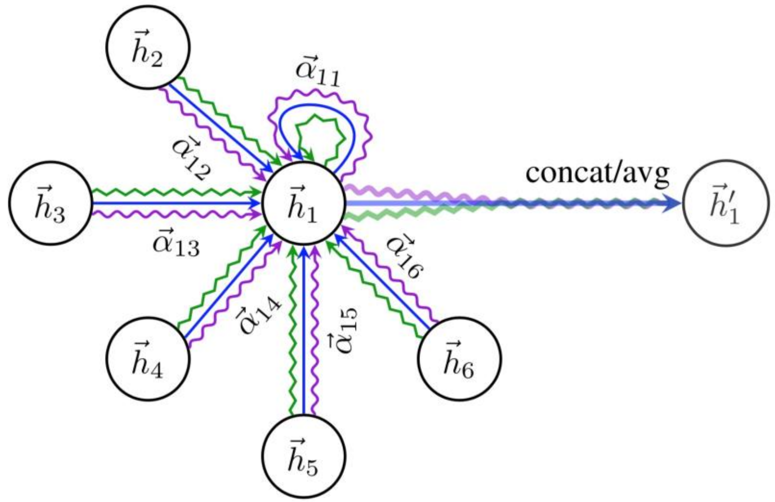


Neural Network Based Method

Background: Graph Representation Learning

- Graph Neural Network: a rising method.
  - Design different message passing mechanism between nodes.
  - Capture various kinds of context information on graph.





Graph Neural network is a promising way to model road network.

Background: Motivation

Our idea

- **Graph Neural Network** is able to generate high-quality node representation that capture various characteristics of graph.

- **Road Network** is a kind of typical graph data.

- **Our idea** is to model road network by graph neural network to provide high-quality road representations for down-streaming tasks.

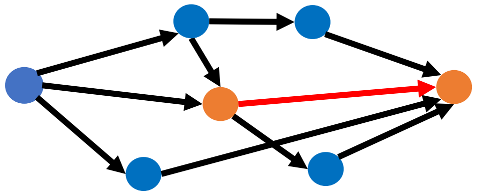
Background: Key Research Problems

- Road network naturally has a hierarchical structure.
  - Transportation hub and commercial area
- Road network is not "small-world".
  - Tending to have long average paths
- It's difficult to model the functional role of a traffic unit based on network structure
  - Determining if a road is shopping mall

Hierarchical Road Network Representation model

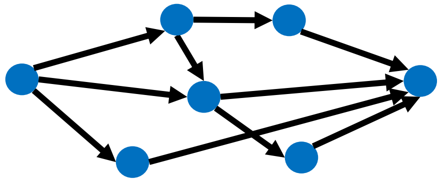
Background: Problem Definition

- Route Segment



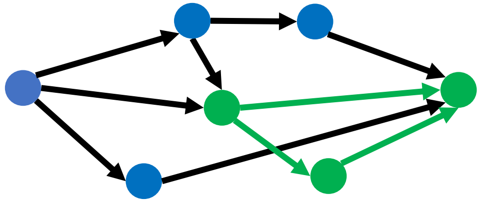
A traffic unit on road network

- Road Network



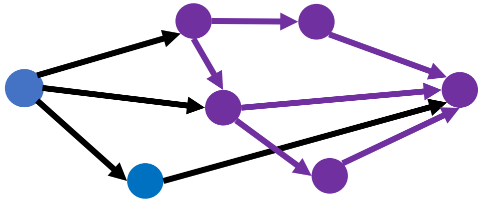
Node: location
Edge: road segment

- Structural Region



A structural region is composed of a set of of spatially connected road segments.

- Functional Zone



A functional zone consists of multiple structural regions.

- Representation Learning on Road Network

Given a road network, we aim to construct the corresponding hierarchical road network.

Background: Review of GCNs and GATs

Graph Convolution Networks

$$\begin{aligned} \boldsymbol{N}^{out} &= \mathrm{GCN}\left(\boldsymbol{N}^{in}, \boldsymbol{A}\right), \\ \boldsymbol{N}^{out} &= \boldsymbol{D}^{-\frac{1}{2}} \boldsymbol{A} \boldsymbol{D}^{-\frac{1}{2}} \boldsymbol{N}^{in} \boldsymbol{W}_2, \end{aligned}$$

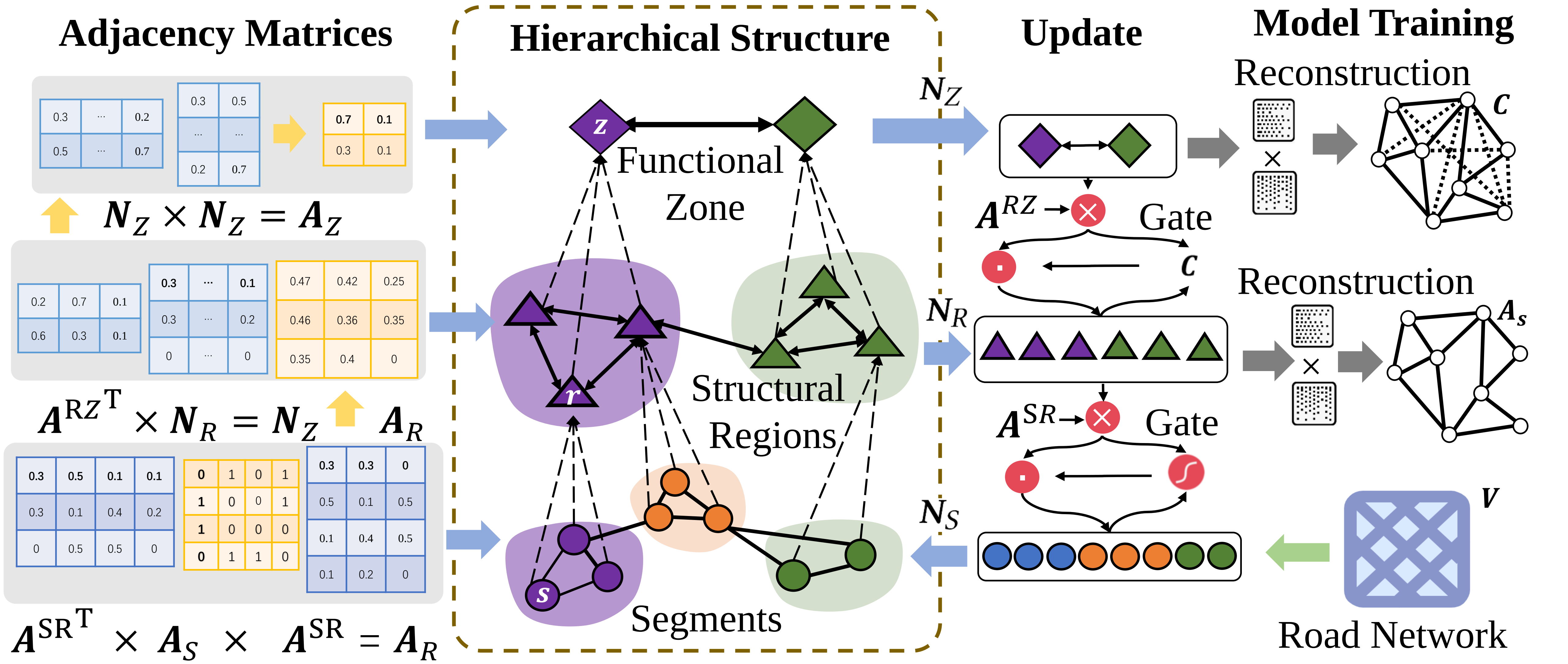
Takes a weighted average of neighbor representations according to adjacent matrix

Graph Attention Networks

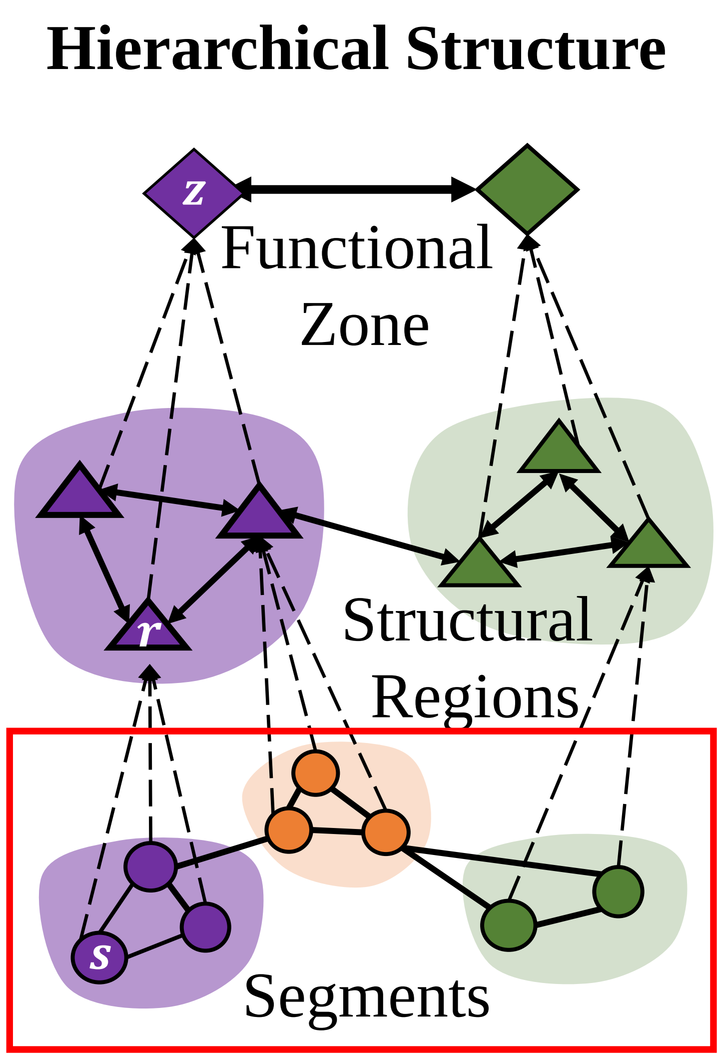
$$\begin{aligned} \boldsymbol{N}^{out} &= \mathrm{GAT}\left(\boldsymbol{N}^{in}, \boldsymbol{A}\right), \\ \boldsymbol{n}_i^{out} &= \sum_{j \in \mathcal{A}_i} \alpha_{i,j} \boldsymbol{n}_j^{in} \boldsymbol{W}_2, \\ \alpha_{i,j} &= \frac{\exp\left(\boldsymbol{w}_1^\top \left(\boldsymbol{W}_1 \boldsymbol{n}_i^{in} + \boldsymbol{W}_1 \boldsymbol{n}_j^{in}\right)\right)}{\sum_{j \in A_i} \exp\left(\boldsymbol{w}_1^\top \left(\boldsymbol{W}_1 \boldsymbol{n}_i^{in} + \boldsymbol{W}_1 \boldsymbol{n}_j^{in}\right)\right)}, \end{aligned}$$

Calculate the weight of neighbor node by attention mechanism

HRNR: Overall



HRNR: Contextual Embedding



- Embedding Rich Context Information

$$v_{s_i} = v_{ID} \| v_{RT} \| v_{LN} \| v_{SL} \| v_{LL},$$

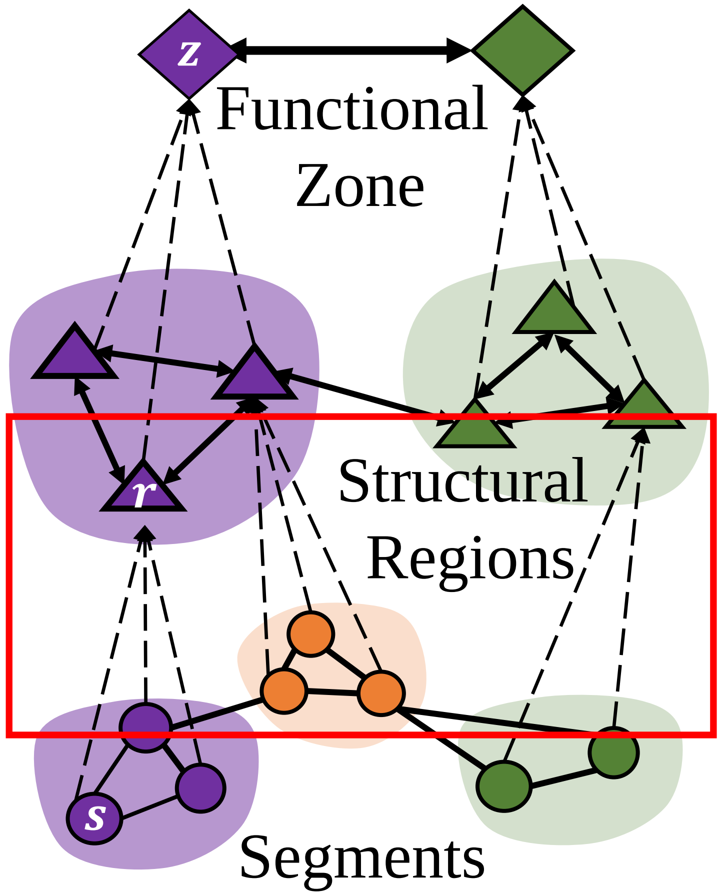
ID, lane number, segment length, longitude and latitude.

- Initializing the graph node embedding

$$N_S^{(0)} \leftarrow V,$$

HRNR: Modeling Structural Regions

Hierarchical Structure



- Constructing Structural Regions by Spectral Clustering

$$M_1[s,r] = \begin{cases} 1 & s \in r, \\ 0 & other. \end{cases}$$

Membership matrix generated by spectral clustering.

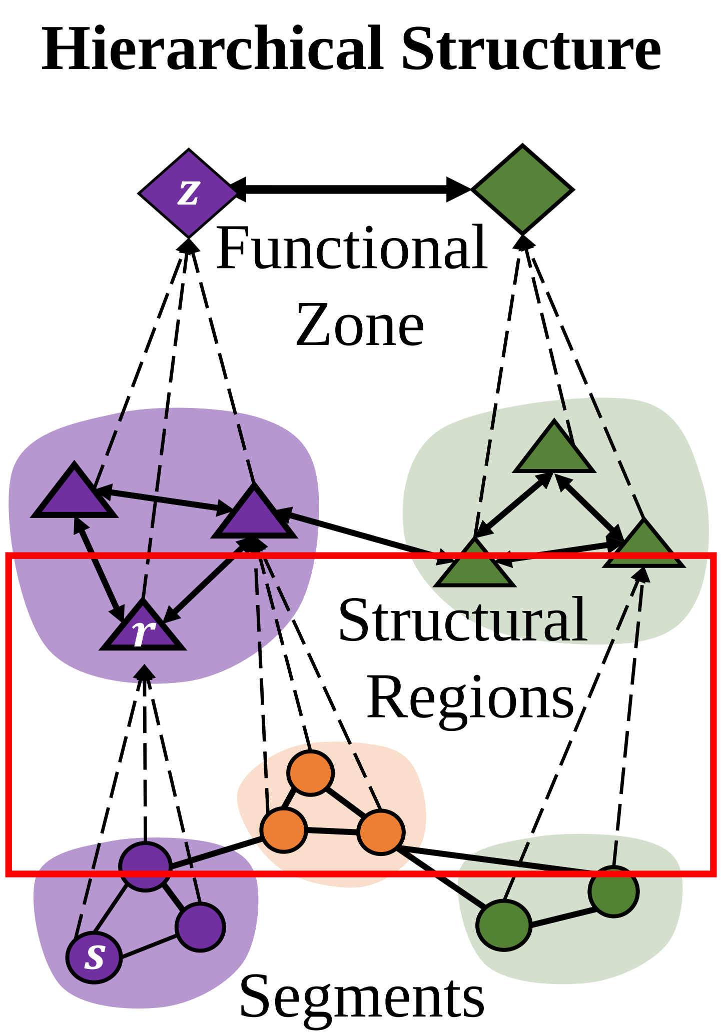
- Learning Region Representations with Assignment Matrix

$$W_1 = \mathrm{GAT}(V, A_S), \qquad A^{SR} = \mathrm{softmax}(M_1 \odot W_1),$$

$$N_R = A^{SR\top} N_S, \qquad A_R = A^{SR\top} \cdot A_S \cdot A^{SR}.$$

Generate region representations N_R and adjacency matrix A_R for region nodes.

HRNR: Modeling Structural Regions



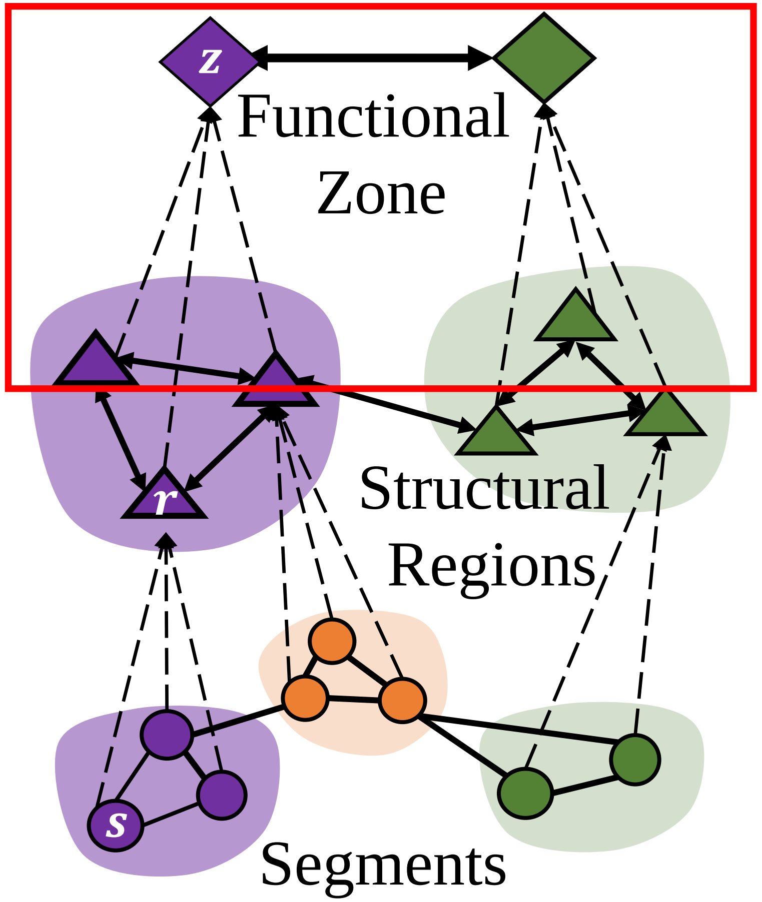
- Learning Assignment Matrix by Network Reconstruction.

Our core idea is to utilize region representations to fit segment representations based on assignment matrix, and reconstruct the road network with the approximated segment representations

$$
\begin{aligned}
Loss_1 = & \sum_{s_i, s_j \in S} -A_S[s_i, s_j] \log(\hat{A}_S[s_i, s_j]) \\
& -(1 - A_S[s_i, s_j]) \log(1 - \hat{A}_S[s_i, s_j]).
\end{aligned}
$$

HRNR: Modeling Functional Zones

Hierarchical Structure

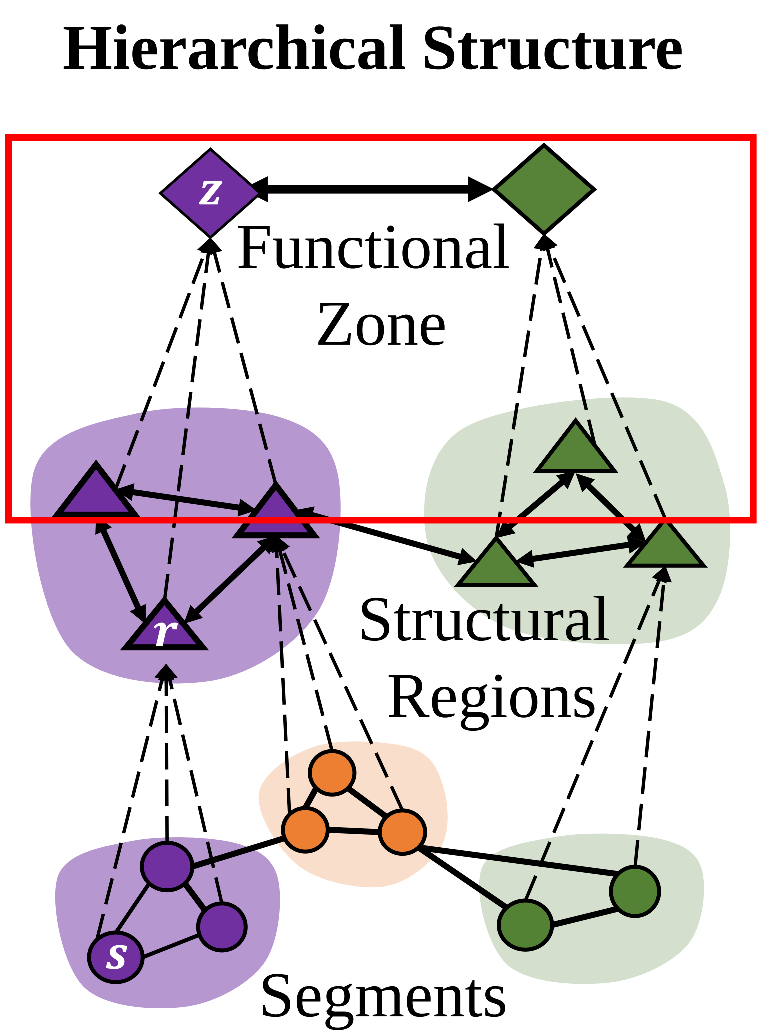


- Learning Zone Representations with Assignment Matrix.

$$
\begin{aligned}
A^{RZ} &= \mathrm{softmax}(M_2), \\
M_2 &= \mathrm{GAT}(N_R, A_R), \\
N_Z &= A^{RZ\top} N_R. \\
A_Z &= \mathrm{RELU}\left(N_Z N_Z^\top - \sigma\right),
\end{aligned}
$$

Generate zone representations N_Z and adjacency matrix A_Z for zone nodes based one region representations.

HRNR: Capturing Functional Characteristics



Constructing connectivity matrix

$$C = A_S + \sum_{j=1}^{\lambda} T^{(j)},$$

C considers the connectivity in terms of both road network structure and human moving behavior.

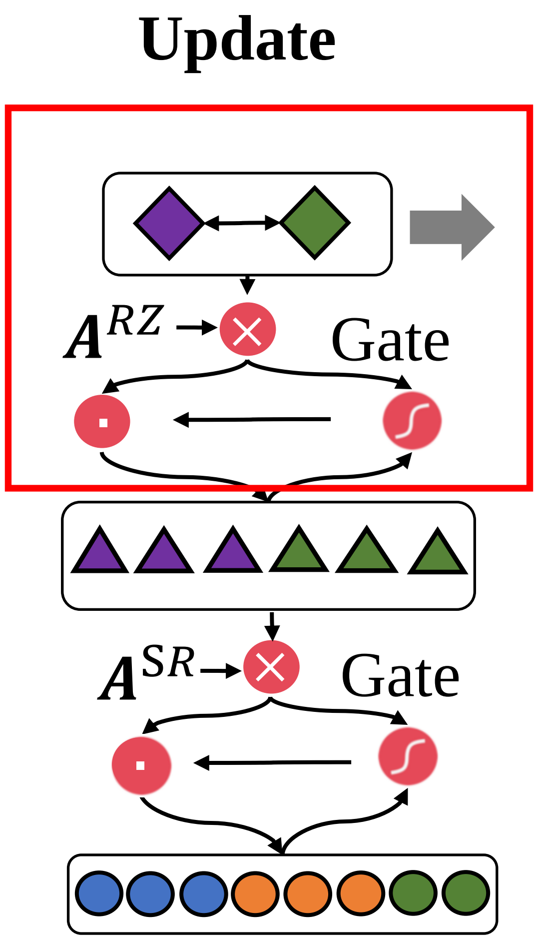
$$\hat{N}_S = A^{SR} A^{RZ} N_Z,$$

$$\hat{C} = \hat{N}_S \hat{N}_S^{\top}.$$

$$Loss_2 = \|C - \hat{C}\|^2,$$

We try to reconstruct the connectivity matrix based one zone representations.

HRNR: Hierarchical Update Mechanism



Zone-level Update.

We update zone representations and prepare them for message passing to the next level.

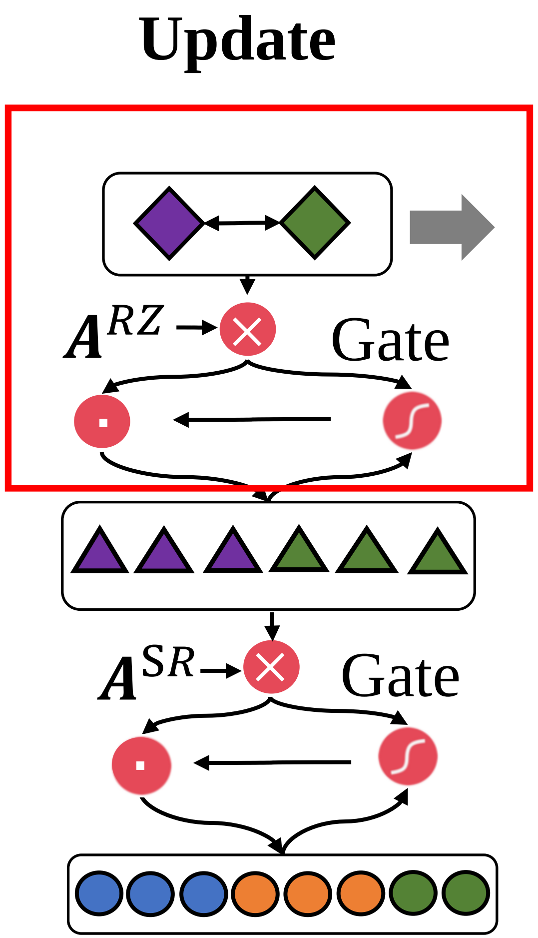
$$\mathbf{N}_Z^{(t+1)} = \mathrm{GCN}\left(\mathbf{N}_Z^{(t)}, \mathbf{A}_Z\right),$$

We adopt a standard Graph Convolutional Network (GCN) to update the zone embedding.

$$\tilde{\mathbf{N}_R}^{(t)} = \mathbf{N}_R^{(t)} + \boldsymbol{g}^{ZR} \odot \left(\mathbf{A}^{RZ}\mathbf{N}_Z^{(t+1)}\right),$$

$$\boldsymbol{g}^{ZR} = \mathrm{sigmoid}\left(\left(\mathbf{N}_R^{(t)} \| (\mathbf{A}^{RZ}\mathbf{N}_Z^{(t+1)})\right) \cdot \boldsymbol{w}_1\right),$$

HRNR: Hierarchical Update Mechanism



Region-level Update.

At the region level, it first updates its own embedding representations by adopting standard GCN.

$$\mathbf{N}_R^{(t+1)} = \mathrm{GCN}\left(\tilde{\mathbf{N}}_R^{(t)}, \mathbf{A}_R\right),$$

We forward the region embeddings to the next level for updating the segment representation.

$$\begin{aligned} \tilde{\mathbf{N}}_S^{(t)} &= \mathbf{N}_S^{(t)} + \mathbf{g}^{RS} \odot \left(\mathbf{A}^{SR}\mathbf{N}_R^{(t+1)}\right), \\ \mathbf{g}^{RS} &= \mathrm{sigmoid}\left(\left(\mathbf{N}_S^{(t)} \| (\mathbf{A}^{SR}\mathbf{N}_R^{(t+1)})\right) \cdot \mathbf{w}_2\right), \end{aligned}$$

Segment-level Update.

$$\mathbf{N}_S^{(t+1)} = \mathrm{GAT}\left(\tilde{\mathbf{N}}_S^{(t)}, \mathbf{A}_S\right),$$

NASR: Model Training

Pretrain

- Optimize Loss_1 and Loss_2 to acquire the assignment matrices.

Apply to Down-streaming Tasks

- We apply the the node embeddings to various downstream application.

Algorithm 1 The training algorithm for the HRNR model.

Input: A trajectory dataset $\mathcal{D}$ and a hierarchical road network $\mathcal{H}$.
Output: Model parameters $\Theta^{(i)}$,$\Theta^{(r)}$, and $\Theta^{(z)}$.
Randomly initialize $\Theta^{(i)}$, $\Theta^{(r)}$ and $\Theta^{(z)}$.
Pre-calculate the connectivity matrix C by Eq. (17).
for *episode* = 1 to epoch **do**
    Calculate region representations $\boldsymbol{N_R}$ by Eq. (7).
    Sample the same number of negative links on $\boldsymbol{A_S}$ as negative samples.
    Perform gradient descent (GD) on Eq. (12) *w.r.t.* $\Theta^{(i)}$, $\Theta^{(r)}$.
    Calculate zone representations $\boldsymbol{N_Z}$ by Eq. (15).
    Sample the same number of low-value links on C as negative samples, and high-value links on C as positive samples.
    Perform gradient descent (GD) on Eq. (20) *w.r.t.* $\Theta^{(i)}$, $\Theta^{(r)}$ and $\Theta^{(z)}$.
end for
return $\Theta^{(g)}$,$\Theta^{(h)}$, $\Theta^{(i)}$.

Experiments: Data Description

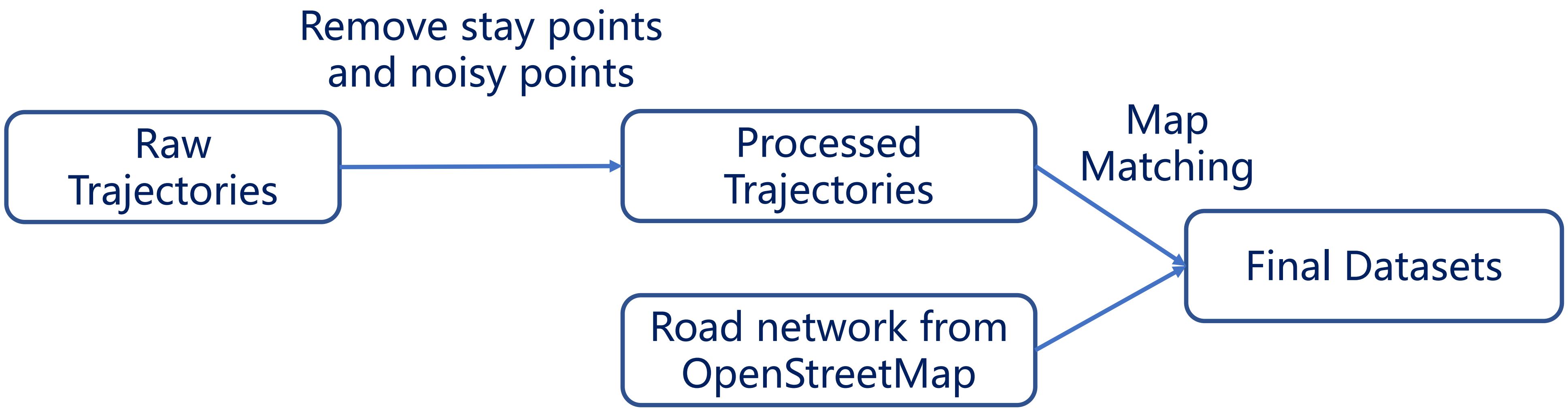


Table 1: Statistics of the three datasets after preprocessing.

Statistics	Beijing	Chengdu	Xi'an
#tpyes	17	13	12
#trajectories	302,654	224,184	493,254
#records	16,040,662	9,632,481	6,672,027
#edges	47,082	8,224	7,341
#road segments	15,500	3,157	2,910
#label	708	303	291
graph diameter	131	71	47
average hop number	48	35	28

Experiments: Metric and Baselines

Evaluation Metrics

- $F1 = \frac{2 * P * R}{P + R}$
- AUC
- $ACC@1$
- $ACC@5$

Benchmarks

- MDW [KDD 2017]: Extended DeepWalk.
- IRN2Vec [SIGSPATIAL 2019]: Road Network Embedding
- GAT [ICLR 2017]: Graph Attention Network
- Geo-GCN [ICLR 2020]: Extended GCN
- DP-GCN [NIPS 2018]: Differentiable graph pooling model.

Experiments: Effectiveness

- We discuss four types of tasks：

  Next Location Prediction, Label Classification, Destination Prediction, Route Planning

Set	Tasks	Next Location Prediction						Tasks	Label Classification					
		MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR	Metric	MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR
BJ	ACC@1	0.357	0.362	0.380	0.387	0.388	**0.413**	F1	0.728	0.732	0.770	0.775	0.772	**0.829**
	ACC@5	0.482	0.491	0.514	0.521	0.522	**0.551**	AUC	0.810	0.804	0.841	0.845	0.844	**0.888**
CD	ACC@1	0.370	0.368	0.385	0.396	0.396	**0.422**	F1	0.689	0.687	0.701	0.713	0.703	**0.748**
	ACC@5	0.503	0.496	0.534	0.540	0.541	**0.567**	AUC	0.692	0.690	0.722	0.739	0.733	**0.773**
XA	ACC@1	0.315	0.317	0.333	0.342	0.340	**0.372**	F1	0.619	0.622	0.636	0.643	0.637	**0.685**
	ACC@5	0.449	0.452	0.463	0.471	0.469	**0.503**	AUC	0.624	0.631	0.657	0.670	0.662	**0.716**

Set	Tasks	Destination Predition						Tasks	Route Planning					
		MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR	Metric	MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR
BJ	ACC@1	0.215	0.218	0.233	0.240	0.241	**0.273**	F1	0.269	0.274	0.298	0.300	0.305	**0.329**
	ACC@5	0.313	0.316	0.347	0.350	0.357	**0.396**	EDT	8.742	8.851	8.235	8.151	8.132	**7.851**
CD	ACC@1	0.239	0.235	0.256	0.267	0.263	**0.288**	F1	0.310	0.312	0.330	0.338	0.341	**0.357**
	ACC@5	0.343	0.346	0.375	0.394	0.389	**0.413**	EDT	8.142	8.013	7.869	7.731	7.664	**7.361**
XA	ACC@1	0.201	0.202	0.210	0.222	0.225	**0.251**	F1	0.259	0.254	0.271	0.278	0.282	**0.301**
	ACC@5	0.305	0.304	0.333	0.348	0.351	**0.370**	EDT	9.268	9.163	8.873	8.653	8.532	**8.138**

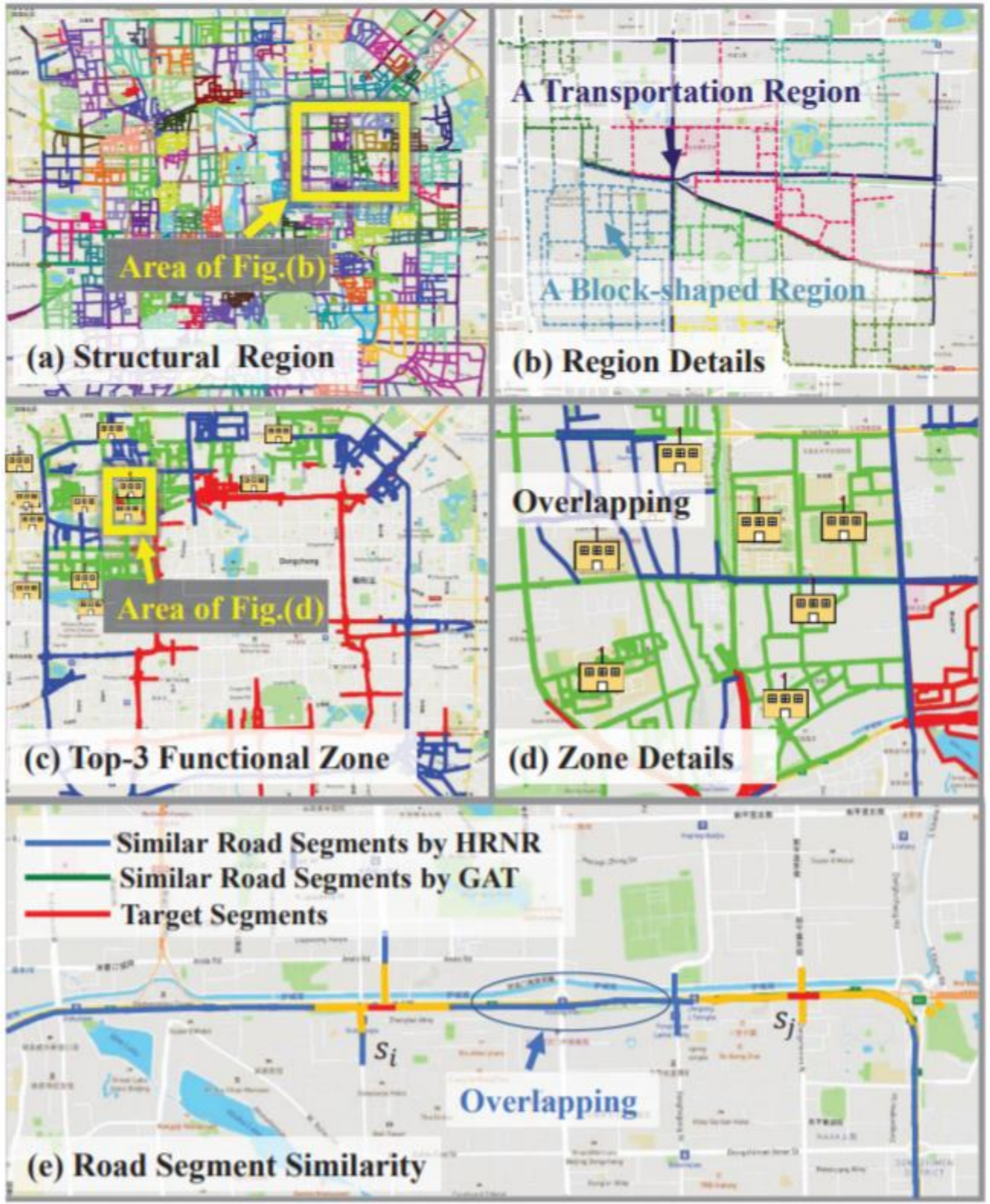
Experiments: Effectiveness

Set	Tasks	Next Location Prediction						Tasks	Label Classification					
Set		MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR	Metric	MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR
BJ	ACC@1	0.357	0.362	0.380	0.387	0.388	**0.413**	F1	0.728	0.732	0.770	0.775	0.772	**0.829**
	ACC@5	0.482	0.491	0.514	0.521	0.522	**0.551**	AUC	0.810	0.804	0.841	0.845	0.844	**0.888**
CD	ACC@1	0.370	0.368	0.385	0.396	0.396	**0.422**	F1	0.689	0.687	0.701	0.713	0.703	**0.748**
	ACC@5	0.503	0.496	0.534	0.540	0.541	**0.567**	AUC	0.692	0.690	0.722	0.739	0.733	**0.773**
XA	ACC@1	0.315	0.317	0.333	0.342	0.340	**0.372**	F1	0.619	0.622	0.636	0.643	0.637	**0.685**
	ACC@5	0.449	0.452	0.463	0.471	0.469	**0.503**	AUC	0.624	0.631	0.657	0.670	0.662	**0.716**

Set	Tasks	Destination Predition						Tasks	Route Planning					
Set		MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR	Metric	MDW	IRN2vec	GAT	Geo-GCN	DP-GCN	HRNR
BJ	ACC@1	0.215	0.218	0.233	0.240	0.241	**0.273**	F1	0.269	0.274	0.298	0.300	0.305	**0.329**
	ACC@5	0.313	0.316	0.347	0.350	0.357	**0.396**	EDT	8.742	8.851	8.235	8.151	8.132	**7.851**
CD	ACC@1	0.239	0.235	0.256	0.267	0.263	**0.288**	F1	0.310	0.312	0.330	0.338	0.341	**0.357**
	ACC@5	0.343	0.346	0.375	0.394	0.389	**0.413**	EDT	8.142	8.013	7.869	7.731	7.664	**7.361**
XA	ACC@1	0.201	0.202	0.210	0.222	0.225	**0.251**	F1	0.259	0.254	0.271	0.278	0.282	**0.301**
	ACC@5	0.305	0.304	0.333	0.348	0.351	**0.370**	EDT	9.268	9.163	8.873	8.653	8.532	**8.138**

Our proposed model HRNR performs best among the comparison methods.

Experiments: Detailed Analysis



- Learned Regions
- Learned Zones
- It is clear to see that GAT mainly focuses on very close neighbors in spatial position, while our model indeed captures influencing road segments in a long range

Conclusion

- We proposed a hierarchical graph neural network by characterizing the hierarchy "functional zones" → "structural regions" → "road segments".

- We carefully devised two useful reconstruction loss functions to capture both structural and functional characteristics.

- A hierarchical update mechanism was also given tailored to our network architecture.