Graph Neural Networks (GNN)

Wen-Hsiao Peng

National Yang Ming Chiao Tung University (NYCU), Taiwan

July 7, 2021

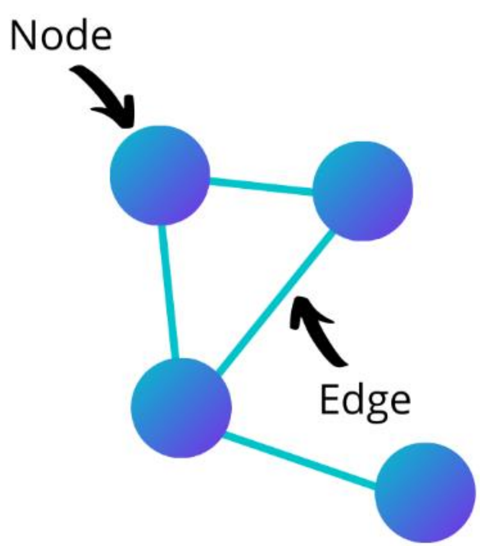
Outline

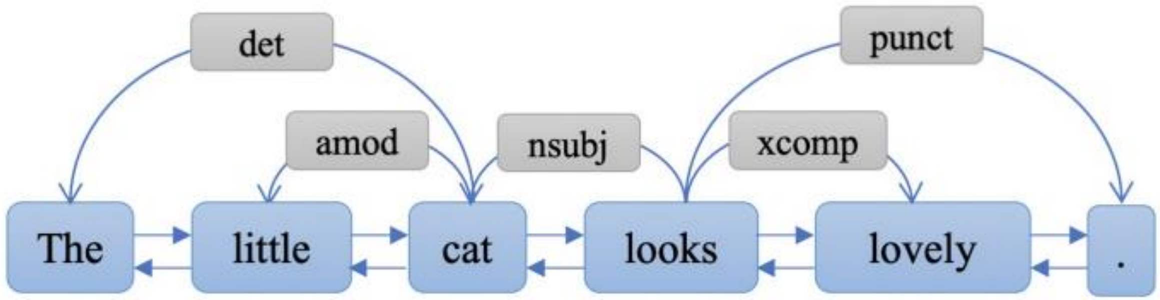
- Introduction to Graph
- Graph Signal Processing
- Graph Neural Networks (GNNs)
  - Spectral-based Convolutional Graph Neural Networks
  - Spatial-based Convolutional Graph Neural Networks
  - Recurrent Graph Neural Networks (RecGNNs)
  - Graph Autoencoders (GAEs)
  - Spatial-temporal Graph Neural Networks (STGNNs)
- Applications

Introduction to Graph

Definition of Graph

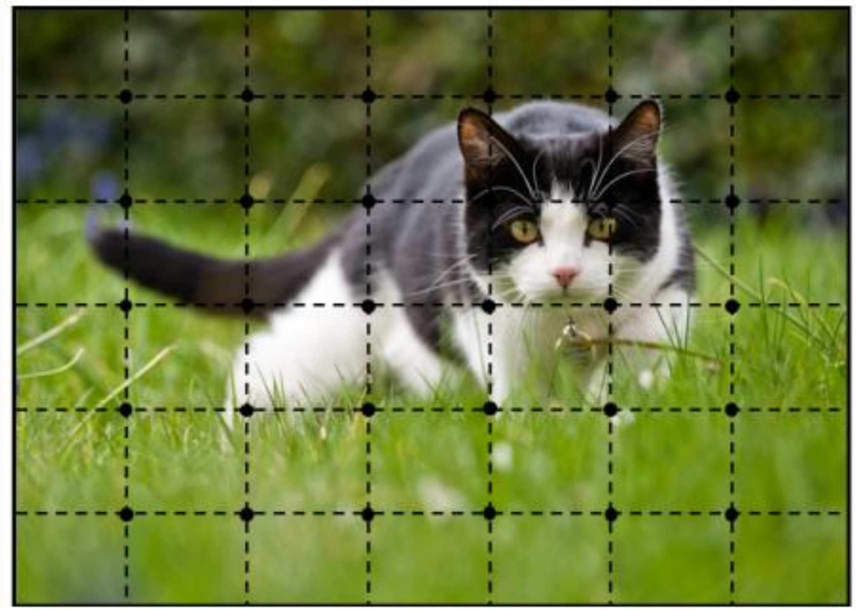
- A collection of nodes $\mathcal{N}$ and edges $\mathcal{E}$
  - **Nodes** contain **data** of interest
  - **Edges** specify **structure**, i.e. how data are related





Words (**nodes**) in a sentence (**graph**)

Graph: More Examples



Roads (**nodes**) in a map (**graph**)

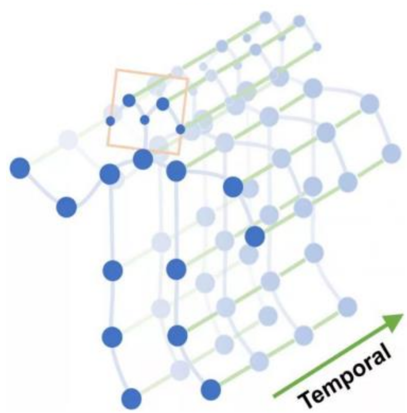
Pixels (**nodes**) in an image (**graph**)

Graph structure can be irregular!

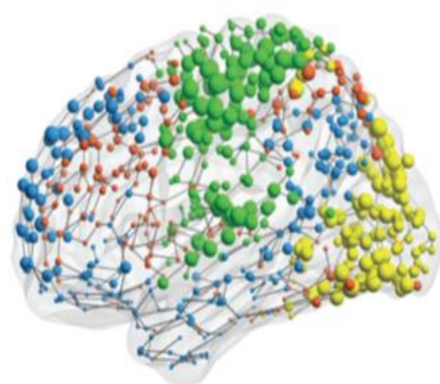
Why Graph?

- Many real-world data come in the form of **graphs**, where **data** (nodes) are related by a **network** (edges)

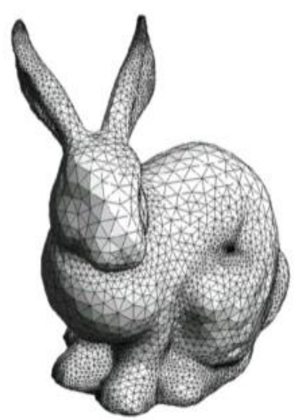
Social networks



Skeleton



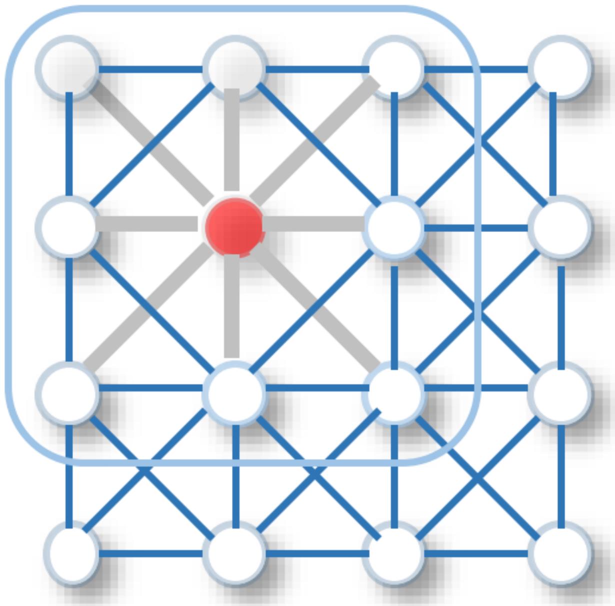
Functional networks



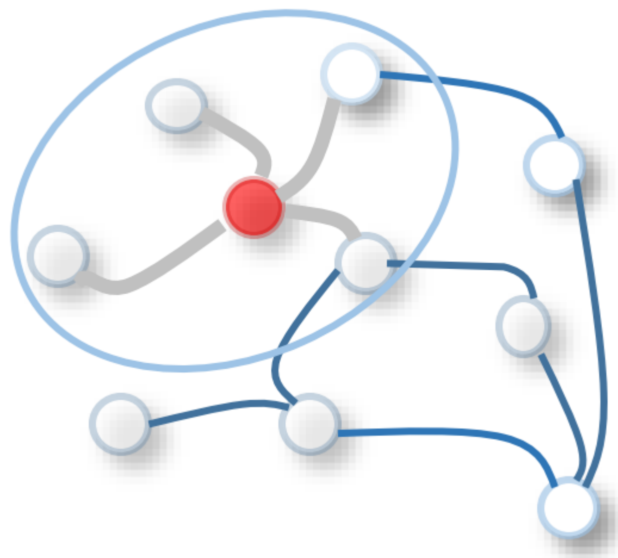
3D shapes

2-D vs. Graph Convolution

Neighbors of a node are ordered and fixed in size



Neighbors of a node are unordered and variable in size



Applying 2-D convolution to graph data becomes difficult!

Wu et al., “A Comprehensive Survey on Graph Neural Networks,” arXiv, 2019

2-D Convolution

- Locality – kernels with a **compact** support
- Stationarity – **space-invariant** kernels
- Multi-scale – **convolution** with **stride and pooling**

Suitable for data (e.g. images, videos) that have these properties!

Graph Convolution

- How to define the notion of **convolution on graph**?

  → Graph signal processing (spectral graph theory)

- How to **downsample and pool graph data**?

  → Clustering on graph (graph theory)

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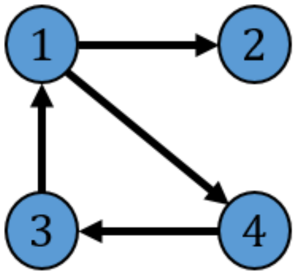
Terminology

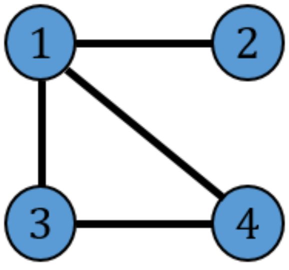
- A graph is represented as $G = (V, E)$ where

  V is the set of nodes, $\{v_1, v_2, \dots, v_n\}$
  E is the set of edges, $\{e_{ij} \mid e_{ij} = (v_i, v_j)\}$

  - e_{ij}: an edge pointing from v_j to v_i
  - Undirected graph: $e_{ij} \in E \rightarrow e_{ji} \in E$
  - Neighborhood $N(\cdot)$ of node v: $\{u \in V \mid (u, v) \in E\}$



Directed Graph



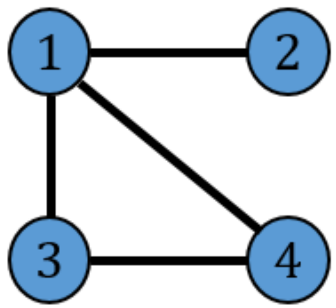
Undirected Graph

Adjacent and Degree Matrices

- Adjacency matrix $\mathrm{A} \in R^{n \times n}$

$$\mathrm{A}_{ij} = 1 \text{ if } e_{ij} \in E, \mathrm{A}_{ij} = 0 \text{ otherwise}$$

$$\mathrm{A} = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$



- Degree matrix $\mathrm{D} \in R^{n \times n}$

$$\mathrm{D} = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix} \qquad \mathrm{D}_{ii} = \sum_{j=1}^{n} \mathrm{A}_{ij}$$

Graph Fourier Transform

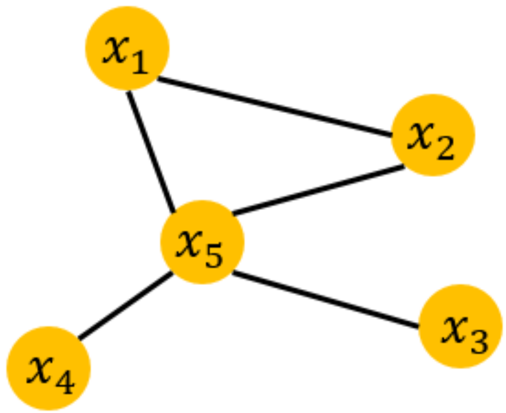
- Graph convolution by graph Fourier transform.

$$x *_G g = \mathcal{F}^{-1}(\mathcal{F}(x) \odot \mathcal{F}(g))$$

number of nodes

- $x \in R^n$ – nodes of graph
- $g \in R^n$ – filter
- $*_G$ – graph convolution
- $\mathcal{F}$ – graph Fourier transform
- $\mathcal{F}^{-1}$ – inverse graph Fourier transform

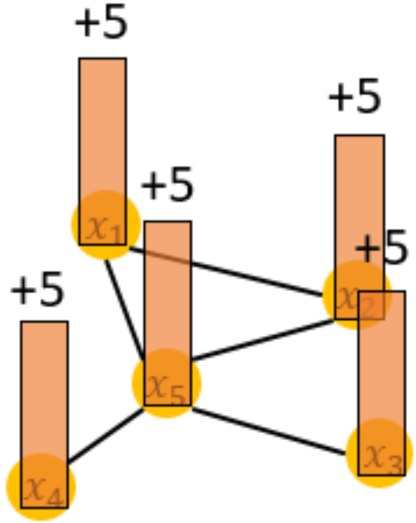
Graph Frequency



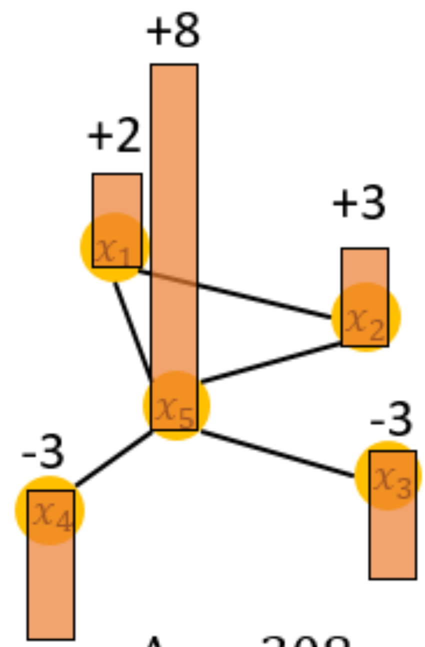
$$\Delta_G = (x_1 - x_2)^2 + (x_1 - x_5)^2 + \cdots$$

$$= \sum_{(u,v)\in E} (x_u - x_v)^2$$

Example:



$\Delta_G = 0$

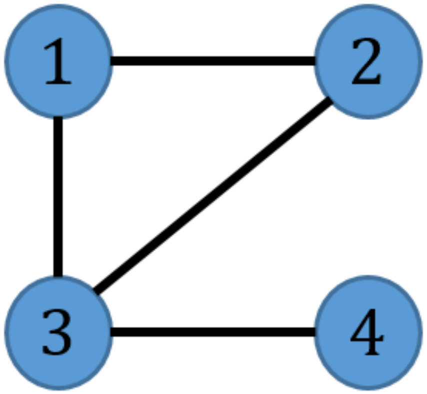


$\Delta_G = 308$

Graph Laplacian

- **Laplacian matrix** $\mathrm{L} = \mathrm{D} - \mathrm{A}$ for **undirected graphs**

$$\mathrm{A} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad \mathrm{D} = \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$



$$\mathrm{L} = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \Rightarrow \frac{1}{2}\mathrm{x}^T \mathrm{L} \mathrm{x} = \sum_{(u,v) \in E} (x_u - x_v)^2$$

Eigen-decomposition of Graph Laplacian

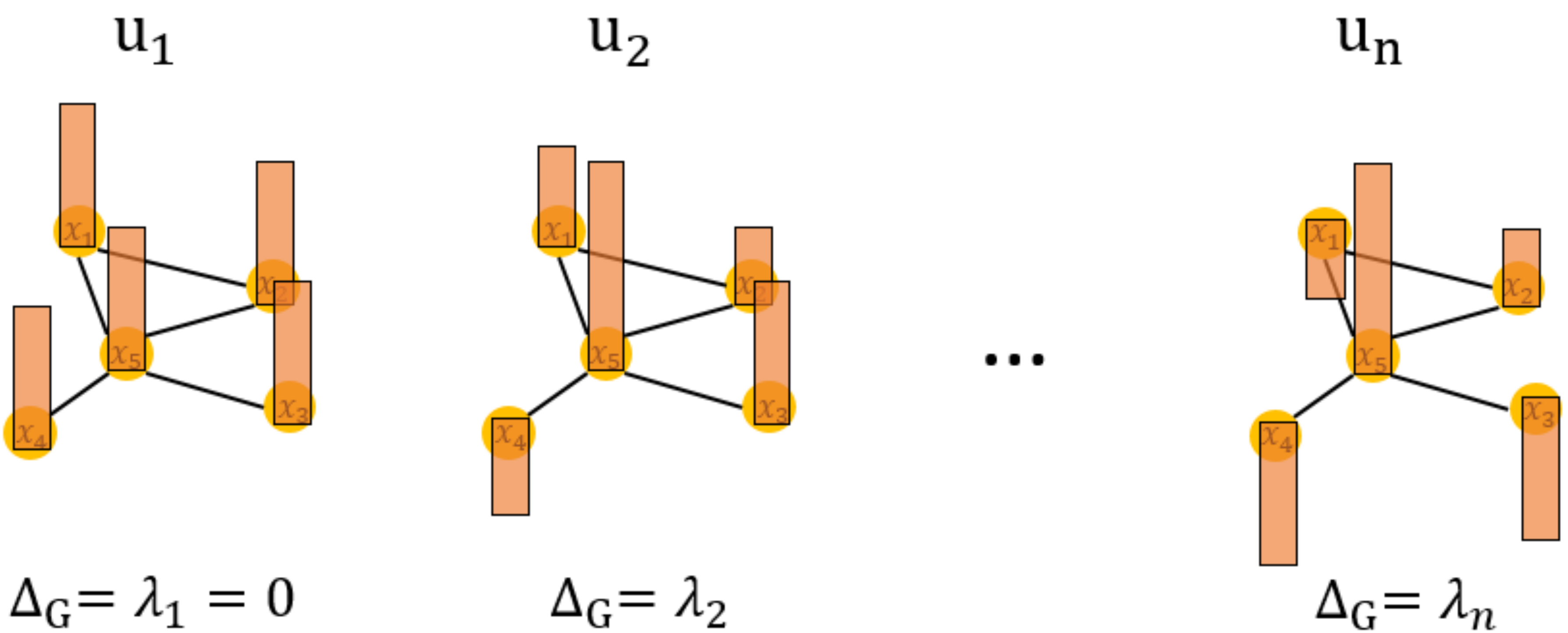
- L is **real**, **symmetric**, and **positive semidefinite**
  - $\mathrm{L} = \mathrm{U}\Lambda\mathrm{U}^T$
  - $\mathrm{U} - [\mathrm{u}_1, \mathrm{u}_2, \ldots, \mathrm{u}_\mathrm{n}]$, $\mathrm{u}_i \in R^n$ and $\mathrm{u}_i^T \mathrm{u}_j = \begin{cases} 1, & \text{if i = j} \\ 0, & \text{otherwise} \end{cases}$
  - $\Lambda - diag([\lambda_1, \lambda_2, \ldots, \lambda_n])$, $\lambda_i \in R$ and $\lambda_1 < \lambda_2 < \cdots < \lambda_n$
- Graph frequency of eigenvectors

$$\mathrm{u}_i^T L \mathrm{u}_i = \mathrm{u}_i^T \lambda_i \mathrm{u}_i = \lambda_i \mathrm{u}_i^T \mathrm{u}_i = \lambda_i$$

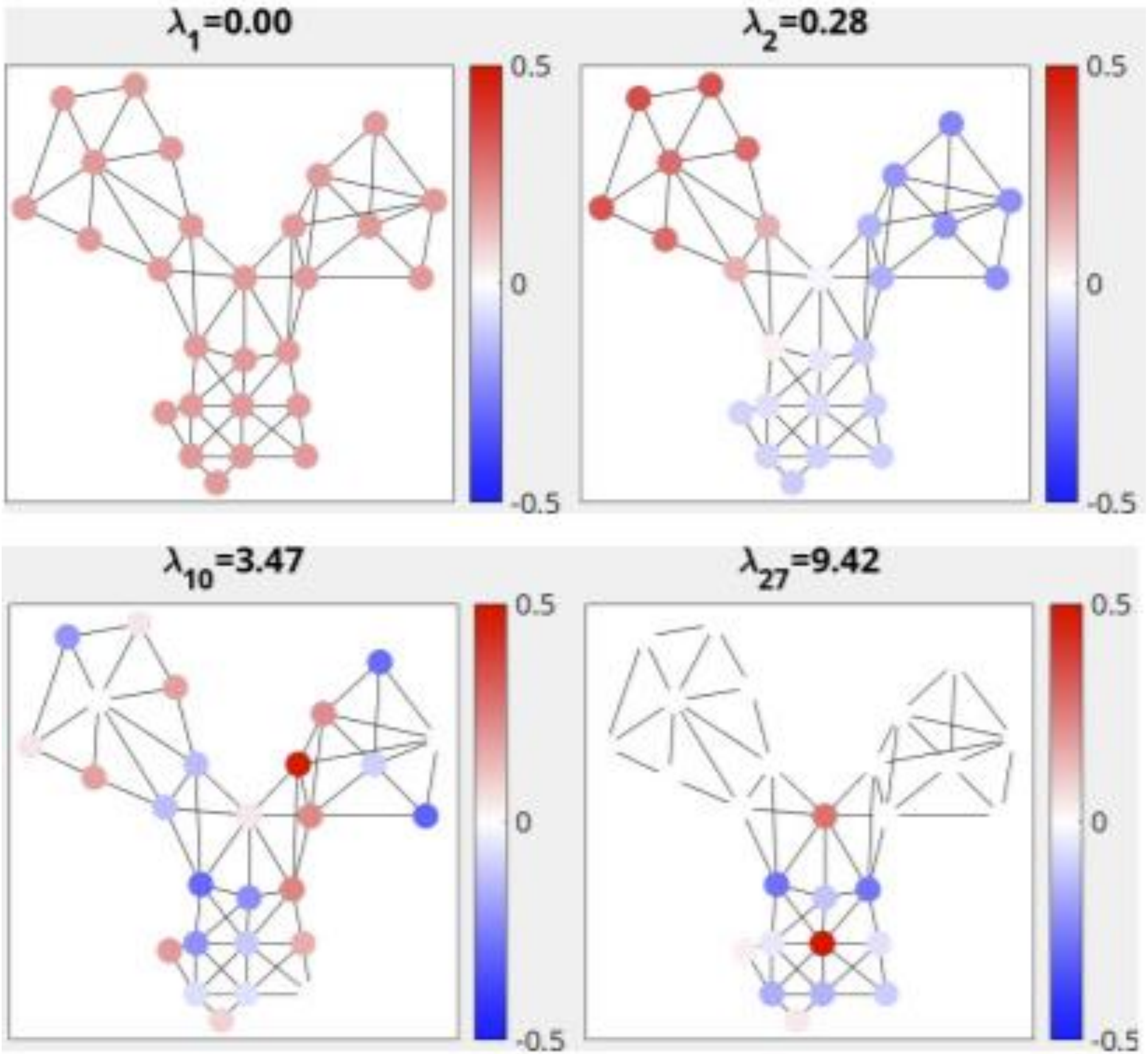
Graph Basis: Eigenvectors of L

$$u_i^T L u_i = u_i^T \lambda_i u_i = \lambda_i u_i^T u_i = \lambda_i$$

$$\lambda_1 < \lambda_2 < \cdots < \lambda_n$$



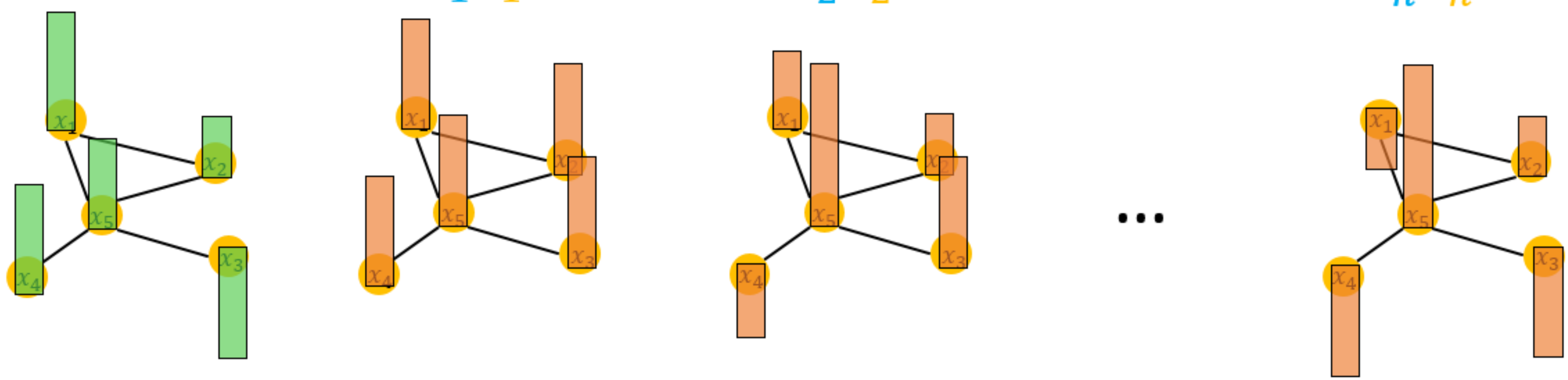
Visualization of Eigenvectors



Graph Transform Coefficients

$$\mathrm{x} = \mathrm{Ix} = \underbrace{\mathrm{U}}_{\text{Graph basis}}\underbrace{\mathrm{U}^T\mathrm{x}}_{\text{Graph Transform Coeff.}}$$

$$\mathrm{x} = \alpha_1 \mathrm{u}_1 + \alpha_2 \mathrm{u}_2 \quad \cdots \quad + \alpha_n \mathrm{u}_n$$



$\Delta_G = \lambda_1 = 0$ $\quad$ $\Delta_G = \lambda_2$ $\quad$ $\Delta_G = \lambda_n$

Graph Convolution

$$\begin{pmatrix}a\\b\end{pmatrix} \odot \begin{pmatrix}c\\d\end{pmatrix} = \begin{pmatrix}c&0\\0&d\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = \begin{pmatrix}ac\\bd\end{pmatrix}$$

- Graph Fourier transform

$$(U^T x \odot U^T g) = g_\theta U^T x$$

$$\mathcal{F}(\mathrm{x}) = \hat{\mathrm{x}} = \mathrm{U}^T\mathrm{x} \quad \text{and} \quad \mathcal{F}^{-1}(\hat{\mathrm{x}}) = \mathrm{U}\hat{\mathrm{x}}$$

- Spectral graph convolution

$$\begin{aligned}\mathrm{x} *_G \mathrm{g} &= \mathcal{F}^{-1}\big(\mathcal{F}(\mathrm{x}) \odot \mathcal{F}(\mathrm{g})\big)\\ &= \mathrm{U}\underline{\big(\mathrm{U}^\mathrm{T}\mathrm{x} \odot \mathrm{U}^\mathrm{T}\mathrm{g}\big)}\\ &= \mathrm{U}\underline{\mathrm{g}_\theta \mathrm{U}^\mathrm{T}}\mathrm{x}\end{aligned}$$

where

$$\mathrm{g}_\theta = diag(U^T g) \text{ is } \textbf{learnable}$$

- Eigen-decomposition requires $O(n^3)$

Spectral-based Graph Convolution

- Inspired theoretically by **graph signal processing**
- Limited to operate on **undirected graphs**
- **Prohibitively expensive** due to **eigenvector decomposition**
- **Poor generalization** to new graphs (i.e. eigenvectors are completely different for different graphs)

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ChebNet: Chebyshev Spectral GNN (1/2)

- Graph convolution

$$\mathrm{x} *_G \mathrm{g} = \mathrm{U} \mathrm{g}_\theta \mathrm{U}^{\mathrm{T}} \mathrm{x}$$

- Approximates g_θ by Chebyshev polynomials

$$\mathrm{g}_\theta \approx \sum_{i=0}^{K} \theta_i T_i(\widetilde{\Lambda})$$

scalar

  - $\widetilde{\Lambda} = 2\,\Lambda/\lambda_{max} - \mathrm{I}$
  - θ_i are learnable
  - $T_i(\widetilde{\Lambda}) = 2\widetilde{\Lambda} T_{i-1}(\widetilde{\Lambda}) - T_{i-2}(\widetilde{\Lambda})$,
  - $T_0(\widetilde{\Lambda}) = \mathrm{I}$ and $T_1(\widetilde{\Lambda}) = \widetilde{\Lambda}$

ChebNet: Chebyshev Spectral GNN (2/2)

- It can be shown that

$$\mathrm{x} *_G \mathrm{g}_\theta \overset{\approx}{\neq} \mathrm{U}\left(\sum_{i=0}^{K} \theta_i T_i(\tilde{\Lambda})\right)\mathrm{U}^T\mathrm{x} = \sum_{i=0}^{K} \theta_i T_i(\tilde{\mathrm{L}})\mathrm{x}$$

  - $\tilde{\mathrm{L}} = 2\ \mathrm{L}/\lambda_{max} - \mathrm{I}$
  - θ_i are learnable
  - $T_i(\tilde{\mathrm{L}})\mathrm{x}$ is localized in space (local feature extraction)
  - $O(Kn) \Rightarrow O(n)$

Graph Convolutional Network (GCN)

- A **first-order approximation of ChebNet** by assuming $K = 1,\ \lambda_{max} = 2,\ \theta = \theta_0 = -\theta_1$

$$\theta_0 T_0(\tilde{L})x$$
$$+\theta_1 T_1(\tilde{L})x$$
$$\cancel{+\theta_2 T_2(\tilde{L})x}$$

$$\text{ChebNet: } \mathrm{x} *_G \mathrm{g}_\theta = \sum_{i=0}^{K} \theta_i T_i(\tilde{\mathrm{L}})\mathrm{x}$$

degree matrix

$$\text{GCN: } \mathrm{x} *_G \mathrm{g}_\theta = \theta \underbrace{\left(\mathrm{I_n} + \mathrm{D}^{-\frac{1}{2}}\mathrm{A}\mathrm{D}^{-\frac{1}{2}}\right)}_{\bar{\mathbf{A}}} \mathrm{x}$$

Adjacency matrix

- $\bar{\mathbf{A}}$x: message-passing and aggregation

Multi-channel GCN (1/2)

- GCN with **multi-channel input/output** and **non-linear activation** f

$$\mathrm{H} = f(\bar{\mathrm{A}}\mathrm{X}\Theta)$$

  - $\mathrm{X} = [\tilde{\mathrm{x}}_1, \tilde{\mathrm{x}}_2, \dots, \tilde{\mathrm{x}}_d] \in R^{n \times d}$ are d input channels on graph
  - $\Theta = [\theta_1, \theta_2, \dots, \theta_s] \in R^{d \times s}$ with θ_i being 1×1 Conv.
  - $\mathrm{H} = \left[\tilde{\mathrm{h}}_1, \tilde{\mathrm{h}}_2, \dots, \tilde{\mathrm{h}}_s\right] \in R^{n \times s}$ are s output channels on graph

Multi-channel GCN (2/2)

- Node output h_v is a **weighted sum** of node **input** $\tilde{\mathrm{x}}_v$ and **its neighbors** $\tilde{\mathrm{x}}_u, u \in N(v)$

$$\mathrm{H}^T = f(\Theta^T \mathrm{X}^T \overline{\mathrm{A}})$$

$$\underbrace{\mathrm{h}_v}_{\text{Output node } v} = f(\Theta^T \underbrace{\sum_{u \in \{N(v) \cup v\}} \overline{\mathrm{A}}_{v,u} \mathrm{x}_u}_{\text{Message-passing and aggregation}})$$

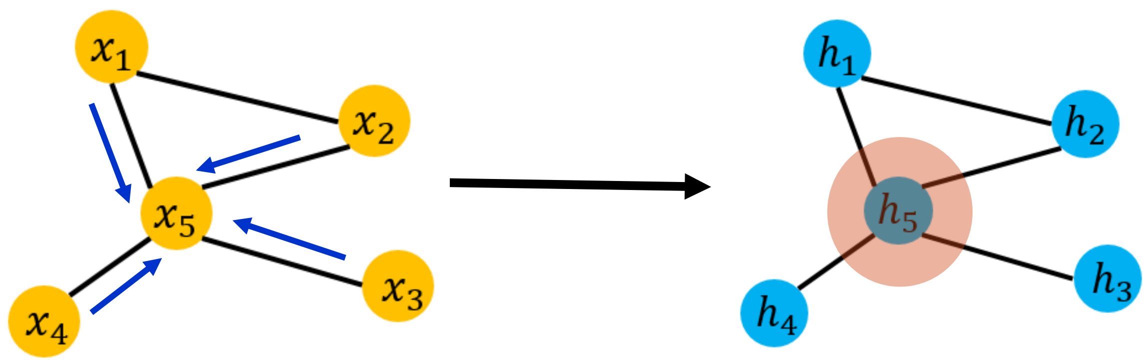
- $\mathrm{x}_u \in \mathrm{R}^d$ is node input u
- $\mathrm{h}_v \in \mathrm{R}^s$ is node output v

Visualization of Multi-channel GCN

$$\mathrm{h}_v = f(\Theta^T \sum_{u\in\{N(v)\cup v\}} \bar{\mathrm{A}}_{v,u}\tilde{\mathrm{x}}_u)$$

Output node v

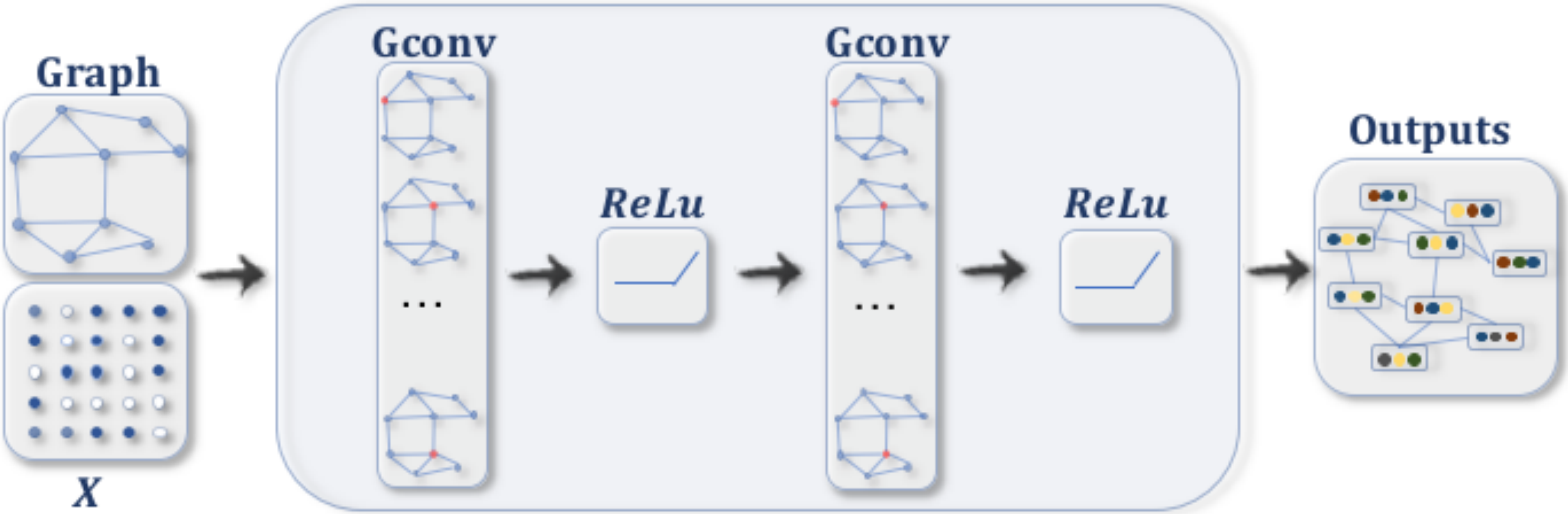
Message-passing and aggregation



Message-passing and aggregation

Message-passing and aggregation is localized on graph!

Composition of GCN Layers

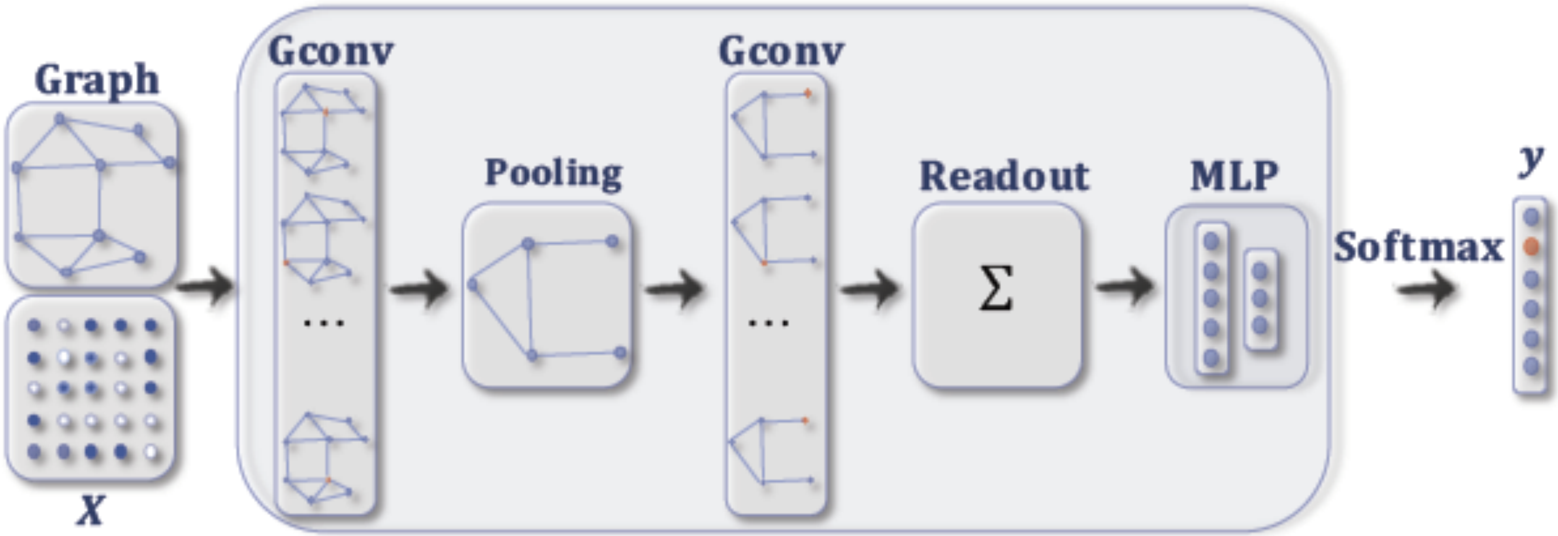


- Each **node input** is a **vector** $\mathrm{x} \in R^d$.
- **Graph input** is a **matrix X** $\in R^{n \times d}$, n is the number of nodes.

Receptive field increases with the number of layers!

Zonghan Wu et al., "A Comprehensive Survey on Graph Neural Networks," IEEE Trans., 2021

GCN with Pooling and Readout

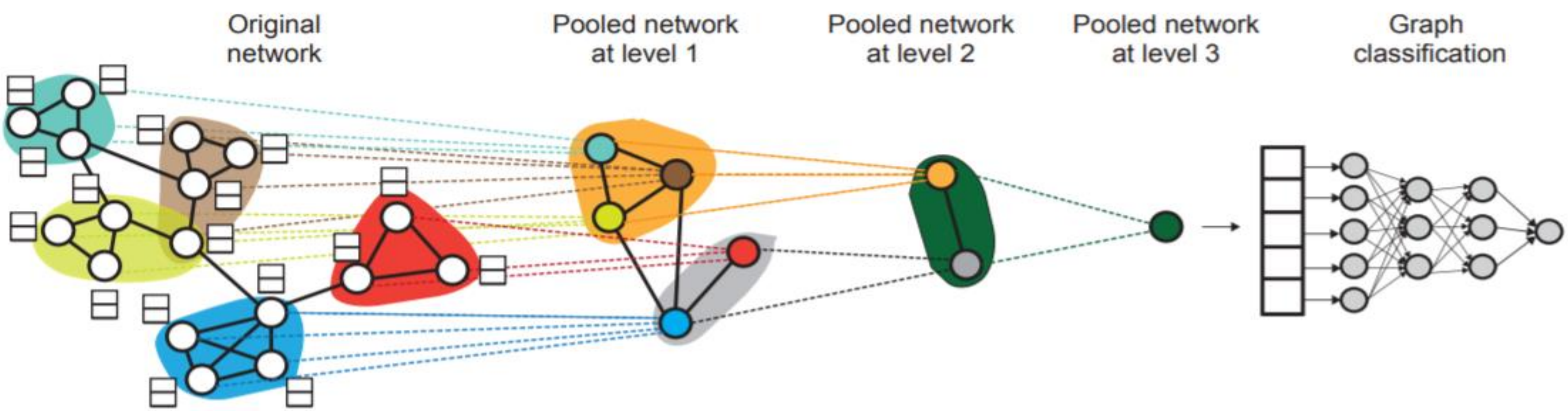


- **Pooling** coarsens a graph into sub-graphs with node representations capturing **higher graph-level representations**
- **Readout** summarizes the final graph by **sum/mean of latent representations** of sub-graphs

Zonghan Wu et al., "A Comprehensive Survey on Graph Neural Networks," IEEE Trans., 2021

Graph Pooling

- Pooling can be achieved by **clustering** the nodes based on **structure information only**



Rex Ying et al., "Hierarchical Graph Representation Learning with Differentiable Pooling," in NIPS, 2018

DiffPool

- To learn **assignment matrix** S for **soft clustering** by involving **both feature and structure** info. with GCN

$$S^{(l)} = \mathrm{softmax}(\mathrm{GNN}_{l,\mathrm{pool}}(A^{(l)}, X^{(l)})) \in R^{n_l \times n_{l+1}}$$

  - n_l is the number of input nodes at layer l
  - n_{l+1} is the number of output clusters for layer $l+1$
  - Softmax is performed row-wise on $S^{(l)}$
  - $S_{ij}^{(l)}$ indicates the probability of node i being clustered to j

Rex Ying et al., "Hierarchical Graph Representation Learning with Differentiable Pooling," NIPS'18

Pooling with Assignment Matrix

- GNN for feature extraction and learning assignment matrix

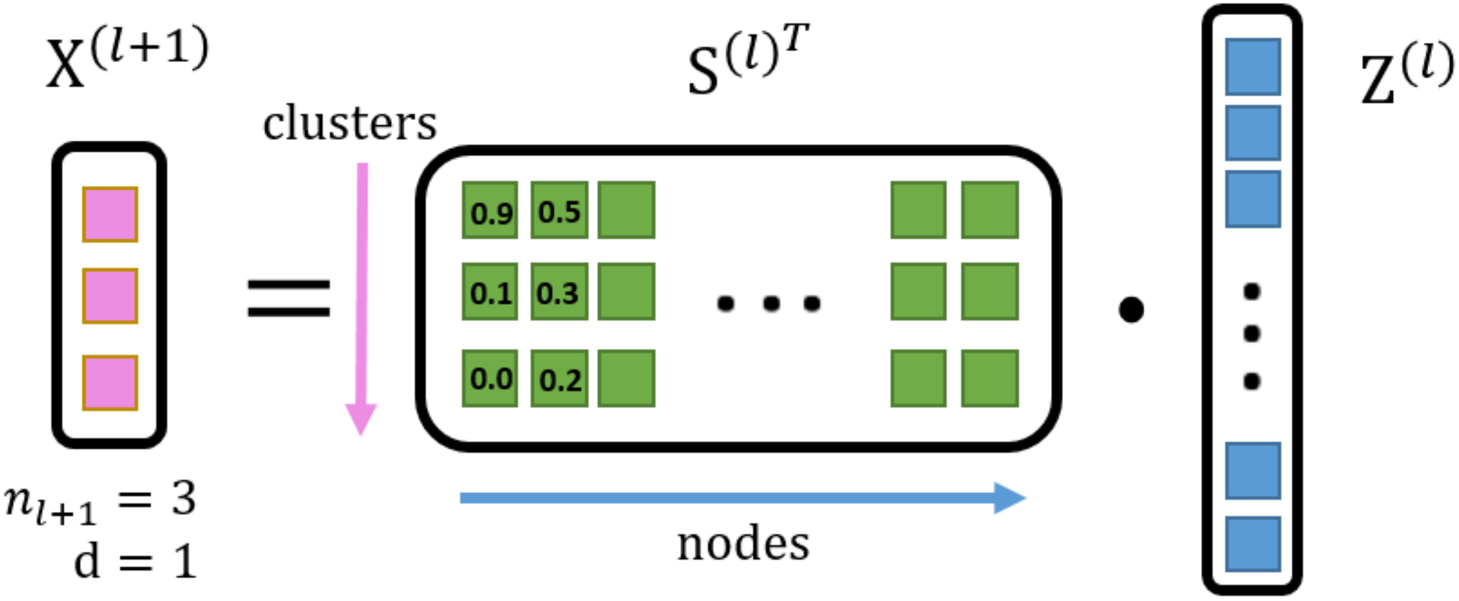
$$Z^{(l)} = \mathrm{GNN}_{l,\mathrm{embed}}(A^{(l)}, X^{(l)}) \in R^{n_l \times d}$$

$$S^{(l)} = \mathrm{softmax}(\mathrm{GNN}_{l,\mathrm{pool}}(A^{(l)}, X^{(l)})) \in R^{n_l \times n_{l+1}}$$

- Pooling

$$X^{(l+1)} = {S^{(l)}}^T Z^{(l)} \in R^{n_{l+1} \times d}$$ # Pooled data

$$A^{(l+1)} = {S^{(l)}}^T A^{(l)} S^{(l)} \in R^{n_{l+1} \times n_{l+1}}$$ # Sub-graph adjacency matrix



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Spatial-based Graph Convolution

- Define **spatial graph convolution** based on **node's spatial relations**

- Convolve a node's representation with its neighbors' to update the node representation

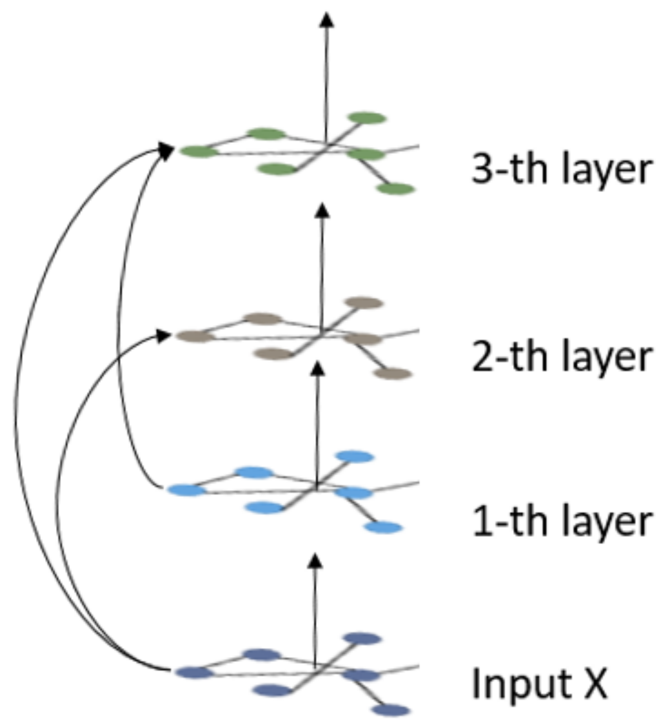
- The idea is the same as **message passing + aggregation**

Wu et al., "A Comprehensive Survey on Graph Neural Networks," arXiv, 2019

Neural Network for Graphs

- Update node v at layer k with its input x_v and its neighbors $\mathrm{h}_u^{(i)}, u \in N(v)$ from all the previous hidden layers $i, i = 1,2, \dots, k-1$

$$\mathrm{h}_v^{(k)} = f(\mathbf{W}^{(k)^T}\mathrm{x}_v + \sum_{u \in N(v)} \sum_{i=1}^{k-1} \mathbf{\Theta}^{(ki)^T} \mathrm{h}_u^{(i)})$$

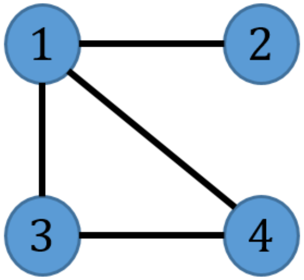


f - activation function
$\mathrm{h}_v^{(k)}$ - the *k*-th latent representation of node *v*
$\mathbf{\Theta}^{(ki)}$ - the 1×1 conv. of the *k*-th layer from the *i*-th layer

Diffusion CNN (1/2)

- Graph convolution as a **diffusion process**

$$\mathbf{H}^{(k)} = f(\mathbf{W}^{(k)} \odot \mathbf{P}^k \mathbf{X})$$



- From a node's perspective → summing information from its neighbors with the transition matrix P

$$\mathrm{P} = \mathrm{D}^{-1}\mathrm{A} \in R^{n \times n}$$

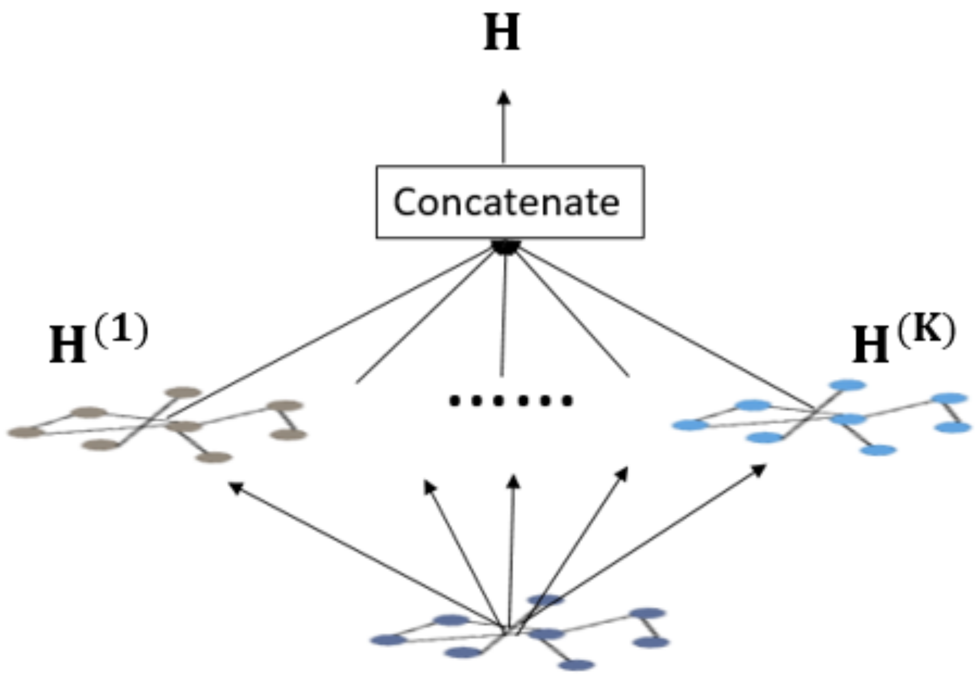
$$A = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}, D = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \quad \mathrm{P} = \begin{bmatrix} 0 & 0.33 & 0.33 & 0.33 \\ 1 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0.5 \\ 0.5 & 0 & 0.5 & 0 \end{bmatrix}$$

Diffusion CNN (2/2)

- Concatenate multi-step propagation results with **variable-size receptive fields**

$$\mathbf{H}^{(k)} = f(\mathbf{W}^{(k)} \odot \mathbf{P}^k \mathbf{X})$$

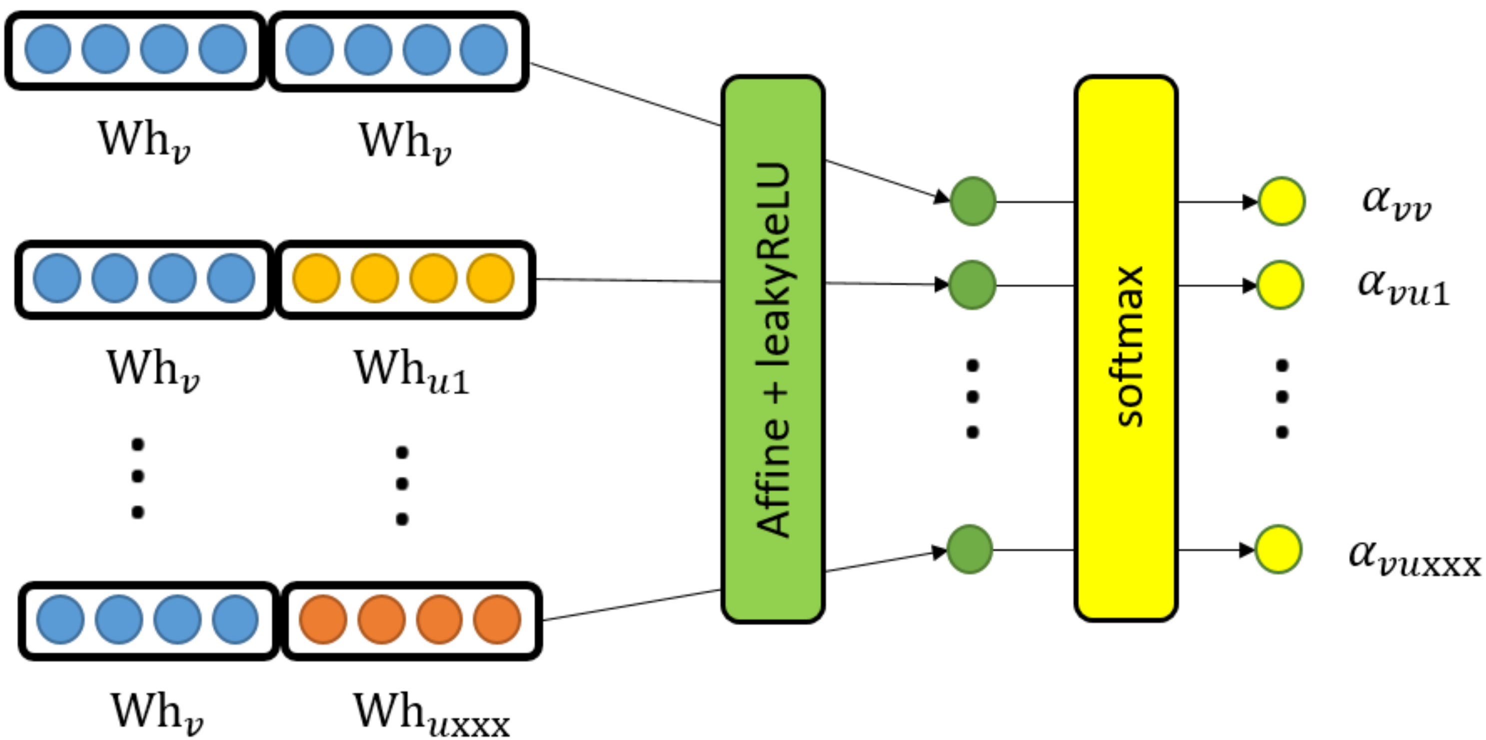
$P^1 \Rightarrow$ diffuse 1 time
$P^2 \Rightarrow$ diffuse 2 times
...
$P^K \Rightarrow$ diffuse K times



Graph Attention Network

$$\mathbf{h}_v^{(k)} = \sigma\Big(\sum_{u \in \mathcal{N}(v) \cup v} \underline{\alpha_{vu}^{(k)}} \mathbf{W}^{(k)} \mathbf{h}_u^{(k-1)} \Big)$$

Attention weights



Comparison with Spectral-based GNN

- Rely primarily on message passing and aggregation
- Scale to large graphs easily
- Perform computation on a batch of nodes, not whole graph
- Share weights easily across different locations and structures
- Generalize easily to different graphs, e.g. directed graphs

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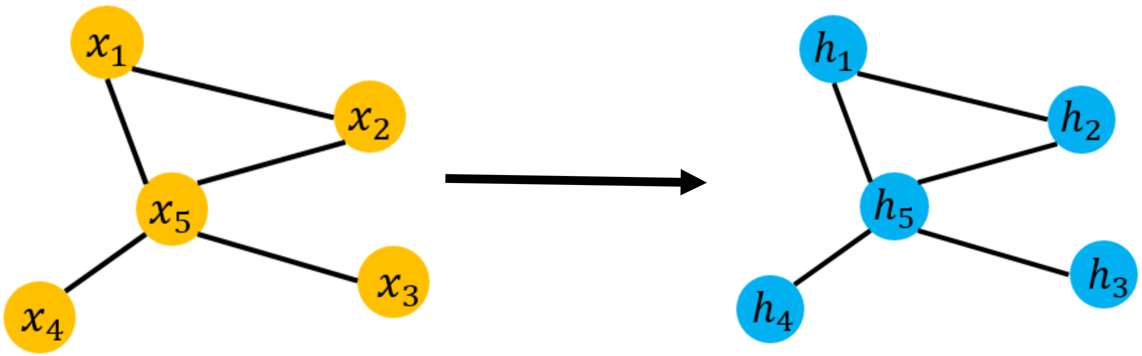
Recurrent Feature Extraction

- **Task**: To extract node feature in a **recurrent** manner



- A node **exchanges information** with its neighbors

$$h_v^{(t)} = \sum_{u \in N(v)} f_W(x_v, x_{(v,u)}^e, x_u, h_u^{(t-1)})$$

Node features Node inputs Node features

Recurrent Feature Extraction

- RecGNNs

$$h_v^{(t)} = \sum_{u \in N(v)} f_w(x_v, x^e_{(u,v)}, x_u\,, h_u^{(t-1)})$$

- f_w must be **contractive** for convergence

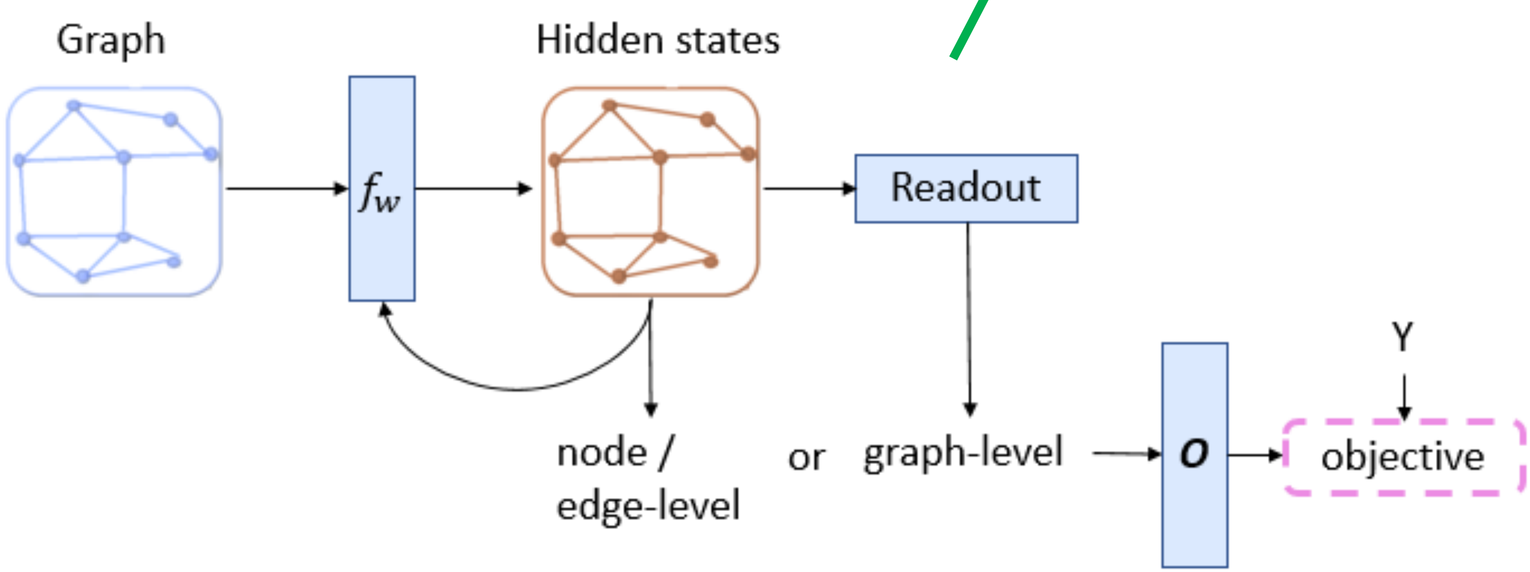
$$\|f_w(x) - f_w(y)\| < \|x - y\| \text{ for any } x, y$$

- Number of iterations for convergence is unknown

Training RecGNNs

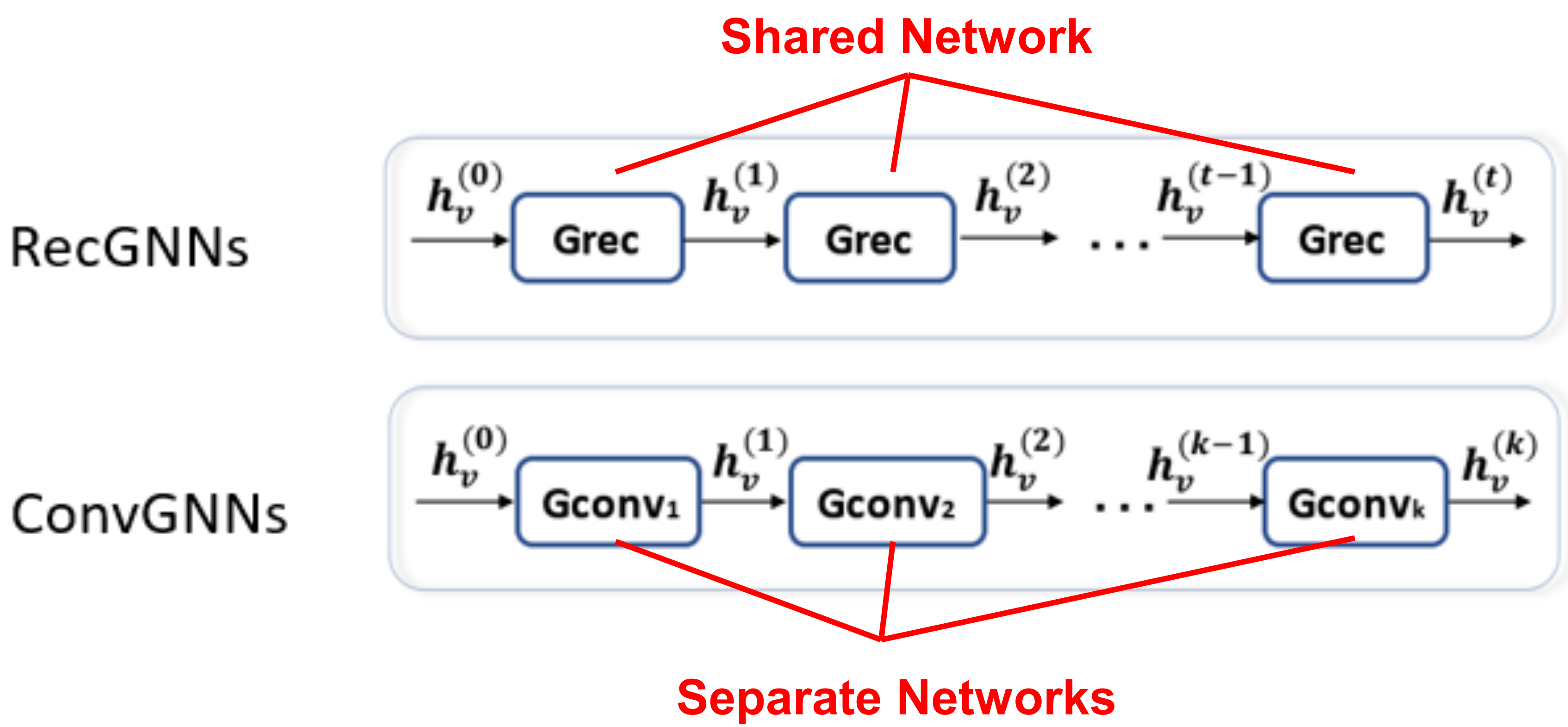
1. Randomly initialize hidden states and networks.
2. Recurrently update hidden states until convergence.
3. Minimize training objective by updating f_w and o networks.
4. Repeat step 2 and 3.

generate graph-level representation
based on hidden stats i.e. sum, concatenate



RecGNNs vs. ConvGNNs

- RecGNNs – propagation is inefficient (t is unknown)
- ConvGNNs – controllable running time (k is known)



Zonghan Wu et al., "A Comprehensive Survey on Graph Neural Networks", IEEE Trans., 2021

Gated Recurrent Neural Networks

- A **fixed number of layers** with training done by BPTT

$$h_v^{(t)} = GRU\left(h_v^{(t-1)}, \sum_{u \in N(v)} \mathrm{W} h_u^{(t-1)}\right)$$

- $h_v^{(0)} = x_v$ is node input

Outline

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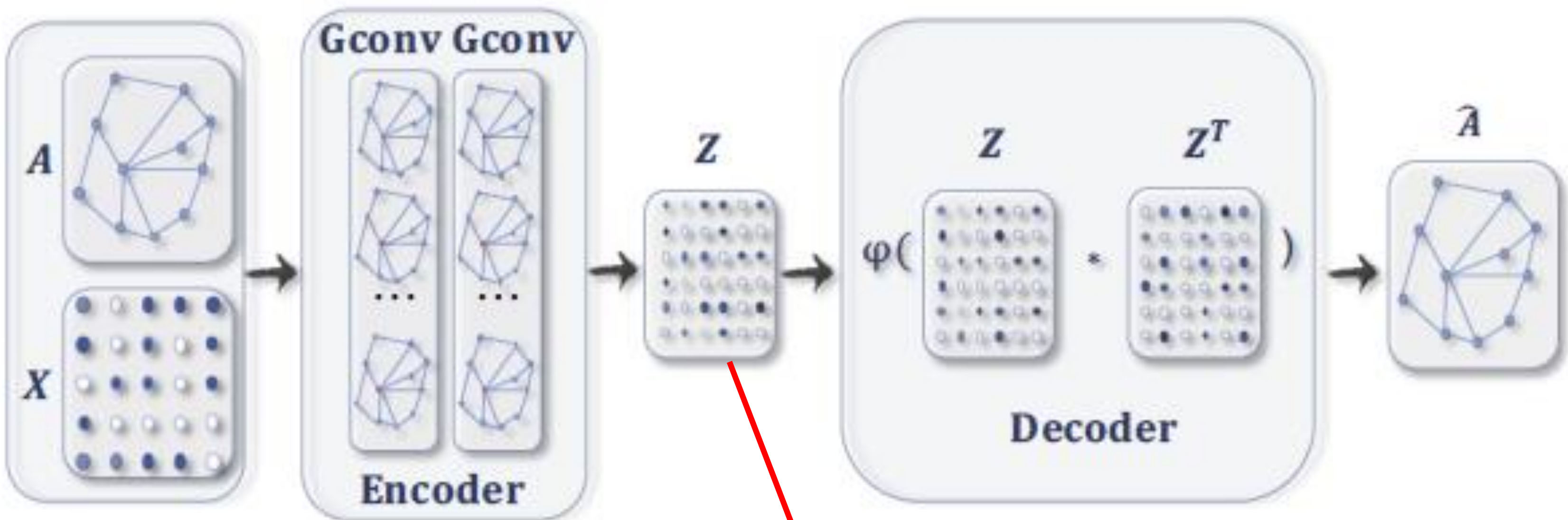
Graph Autoencoders (GAE)

- **<u>Task:</u>** To learn **network embeddings** (i.e. node representations) **for nodes** that preserve **graph topological structure**



Network embeddings

Graph Encoder and Decoder

- Encoder (GNN, MLP, etc) – to **learn network embeddings** by **structure and feature** information

- Decoder (CNN, MLP, etc) – to **predict links between nodes** for reconstructing **adjacency or PPMI matrix**

Positive Pointwise Mutual Information Matrix

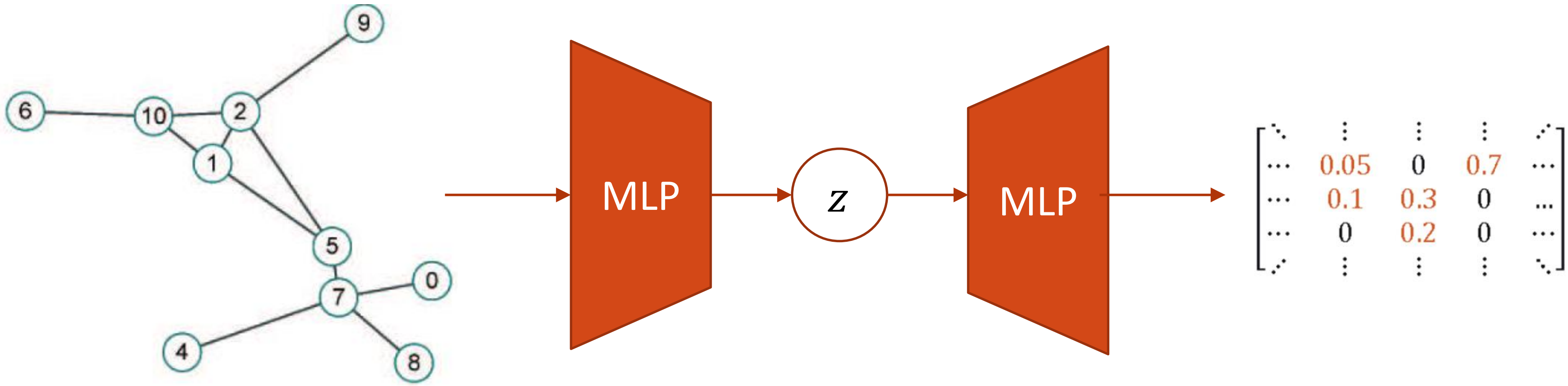
- Capture **mutual information between nodes** by random walks as a specification of the graph structure

$$\mathbf{PPMI}_{v_1,v_2} = max(\log(\frac{count(v_1,v_2)\cdot|D|}{count(v_1)count(v_2)}),0)$$

- $count(v_1)$: the frequency of node v_1 being visited in sampled random walks
- $count(v_1, v_2)$: the frequency of co-occurrence of nodes v_1 and v_2 in sampled random walks

Deep Neural Network for Graph Representations

Adjacency matrix **Denoising autoencoder** **PPMI matrix**



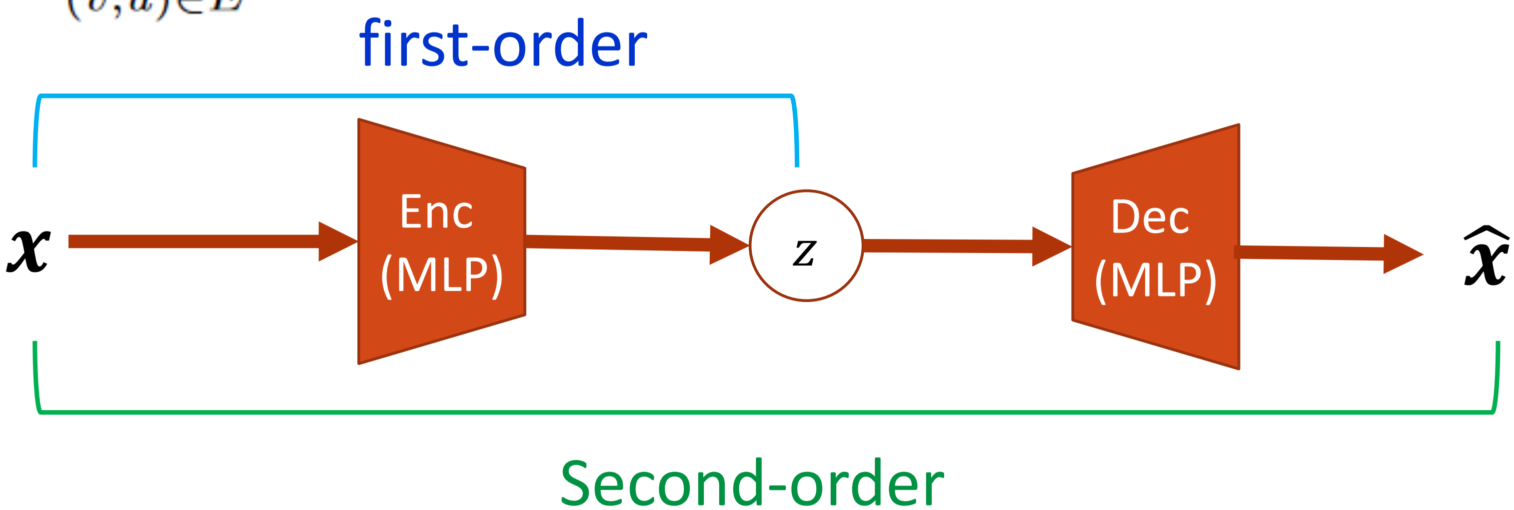
MLP: multi-layer perceptron

Cao et.al, "deep neural networks for learning graph representations," in AAAI, 2016.

Structural Deep Network Embedding

- To preserve the node **first-order** and **second-order** proximity

$$L_{1st} = \sum_{(v,u)\in E} A_{v,u} ||enc(\mathbf{x}_v) - enc(\mathbf{x}_u)||^2$$

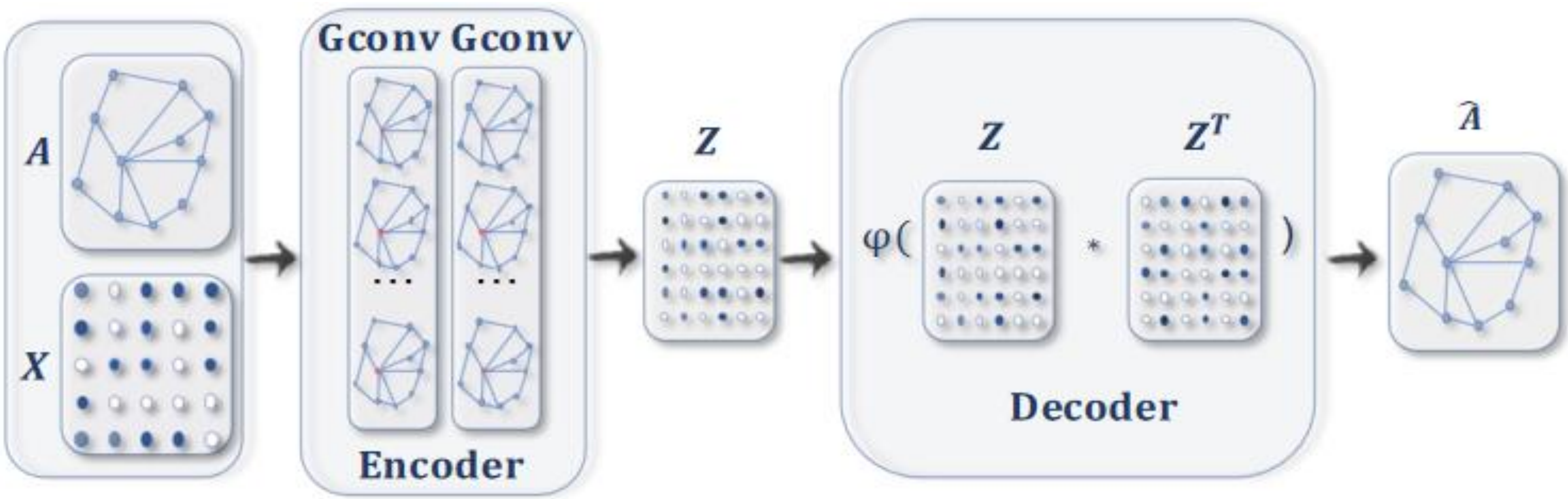


$$L_{2nd} = \sum_{v \in V} ||(dec(enc(\mathbf{x}_v)) - \mathbf{x}_v) \odot \mathbf{b}_v||^2$$

$$b_{v,u} = 1 \quad \text{if } A_{v,u} = 0$$
$$b_{v,u} = \beta > 1 \quad \text{if } A_{v,u} = 1$$

Graph Autoencoder (GAE*)

- GAE* adopts **2-layered GCN** to leverage both **structure and feature information**



GCN

similarity measure

$$\hat{\mathbf{A}}_{v,u} = dec(\mathbf{z}_v, \mathbf{z}_u) = \sigma(\mathbf{z}_v^T \mathbf{z}_u)$$

Wu et.al, "A Comprehensive Survey on Graph NeuralNetworks," in arxiv, 2019.

Variational Graph Autoencoder

- To learn the **generative distribution** of graph
- Optimize the variational lower bound L

$$L = E_{q(\mathbf{Z}|\mathbf{X},\mathbf{A})}[\log p(\mathbf{A}|\mathbf{Z})] - KL[q(\mathbf{Z}|\mathbf{X},\mathbf{A})||p(\mathbf{Z})]$$

- $q(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{A}) = \prod_{i=1}^{n} q(z_i|\boldsymbol{X},\boldsymbol{A})\,, q(z_i|\boldsymbol{X},\boldsymbol{A}) = N\left(z_i \middle| \mu_i, diag\left(\sigma_i^2\right)\right)$
- $p(\boldsymbol{Z}) = \prod_{i=1}^{n} p(z_i)\,, p(z_i) = N(z_i|0,\boldsymbol{I})$
- $p\left(\boldsymbol{A_{ij}} = 1\middle|z_i, z_j\right) = dec\left(z_i, z_j\right) = \sigma(z_i^T z_j)$

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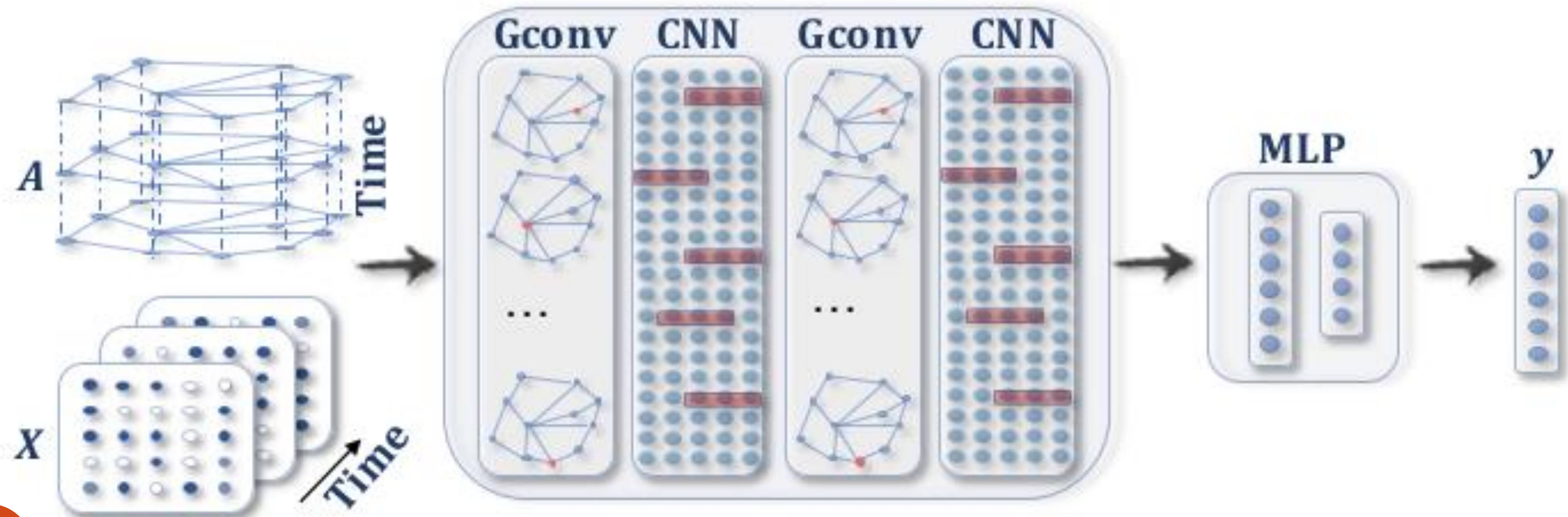
Spatial-temporal Graph Neural Networks

- Real-world graphs are often **dynamic**
- Spatial-temporal Graph Neural Networks (STGNNs)
  - To capture **spatial dynamics via GNN**
  - To capture **temporal dynamics via RNN or CNN**

CNN-based STGNNs

- Apply GCN to aggregate spatial information at individual time instances
- Apply **1D convolution to co-located nodes across time instances** to aggregate temporal information



RNN-based STGNNs

- Recap on RNN

$$H^{(t)} = \sigma\left(WX^{(t)} + UH^{(t-1)} + b\right),$$

  - $X^{(t)} \in R^{n \times d}$ is the node feature matrix at time t

- RNN-based GCN

$$H^{(t)} = \sigma(Gconv\left(X^{(t)}, A; W\right) + Gconv\left(H^{(t-1)}, A; U\right) + b)$$

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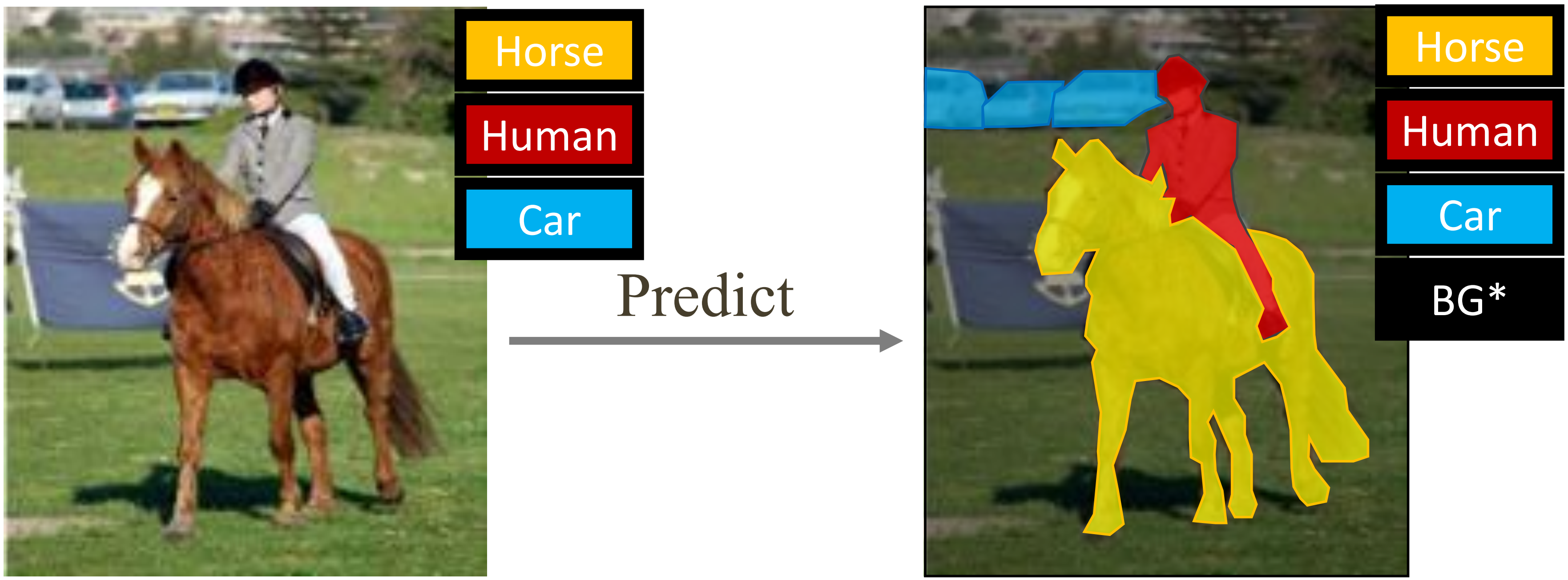
Weakly-Supervised Image Semantic Segmentation Using Graph Convolutional Networks

Shun-Yi Pan, Cheng-You Lu, Shih-Po Lee, and Wen-Hsiao Peng
National Yang Ming Chiao Tung University, Taiwan

IEEE International Conference on Multimedia and Expo (ICME), July 2021.

Task

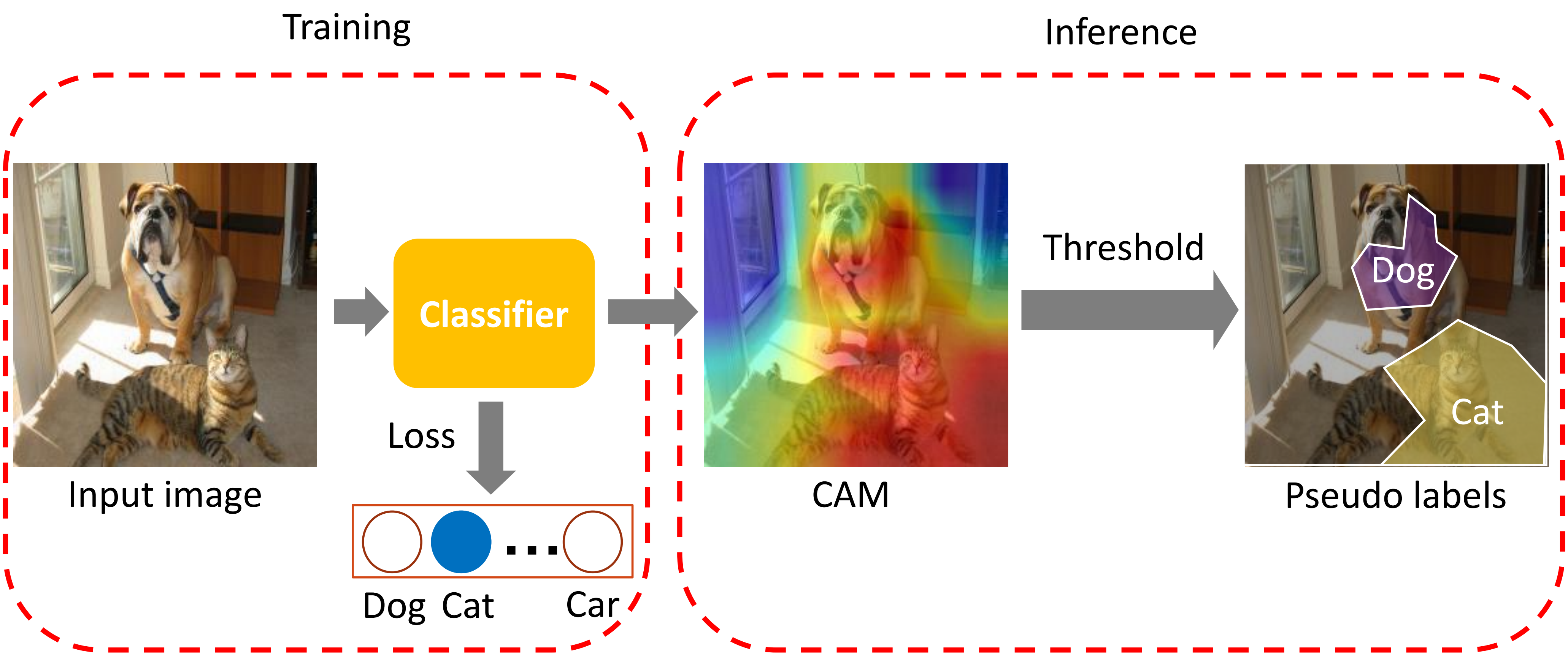
- To classify pixels in images into semantic classes with **image-level annotations**



Input Output

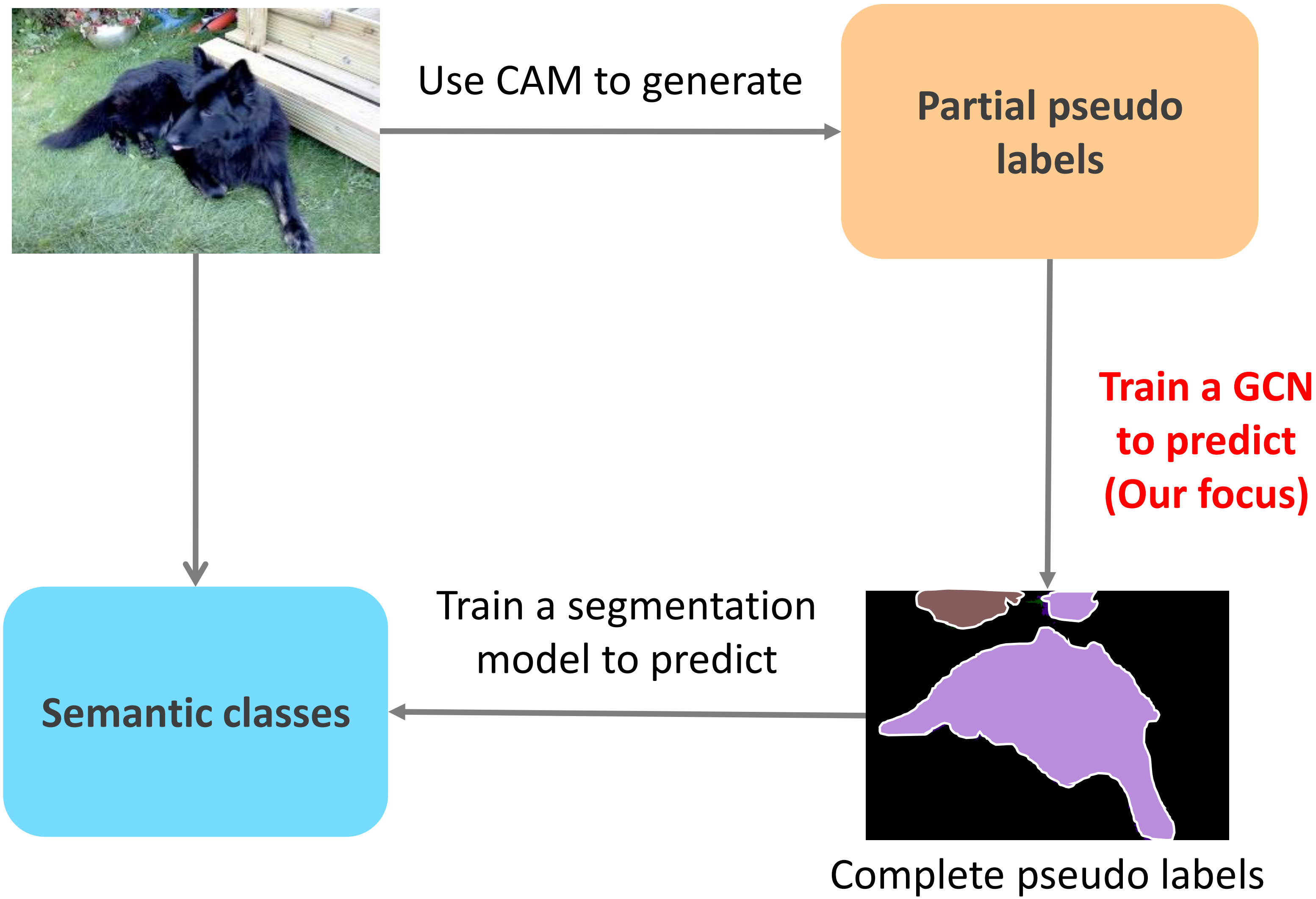
Common Solutions

- Produce **pseudo labels (PLs)** as ground-truth labels
- Use **Class Activation Map** (CAM) to generate PLs



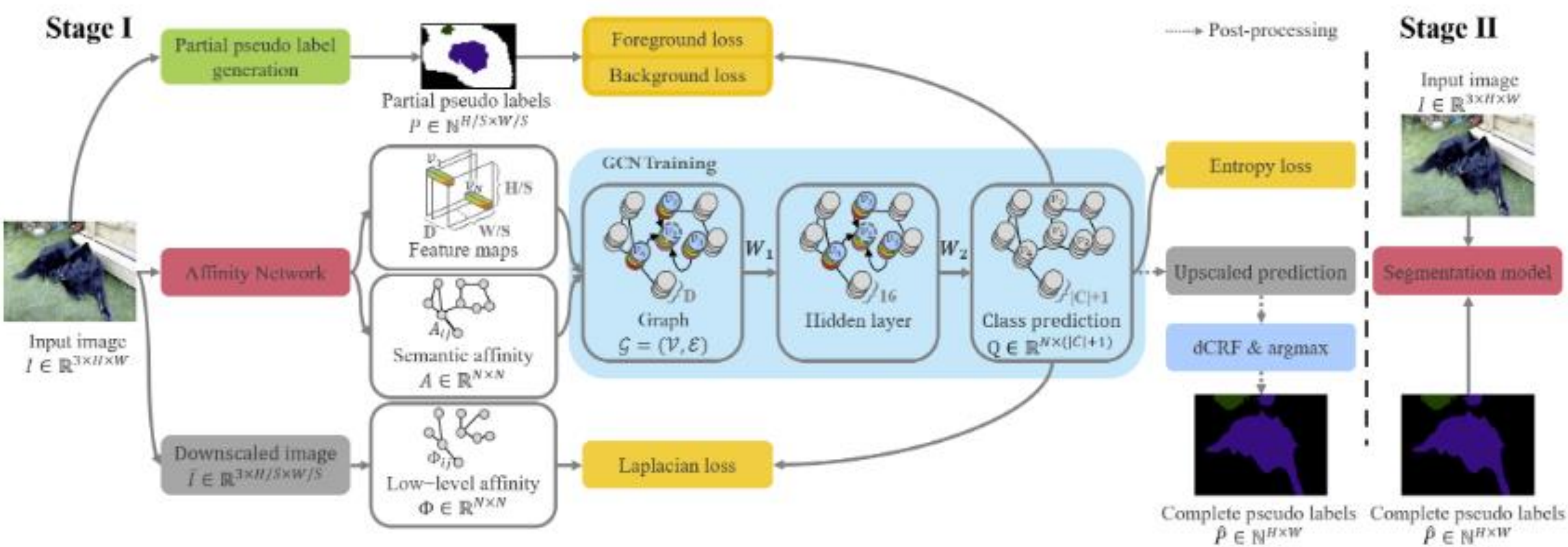
Zhou et al., "Learning deep features for discriminative localization," CVPR'16.

Proposed Method



GCN for Label Propagation

- Use Affinity Network to generate **features of nodes and edges**
- Train a GCN to generate **complete PLs** from **partial PLs**



Loss functions

- Foreground and background loss (**for pixels with pseudo labels**)

$$\ell_{fg} = -\frac{1}{|V_{fg}|}\sum_{i\in V_{fg}} \log(q_i)_{p_i}, \ell_{bg} = -\frac{1}{|V_{bg}|}\sum_{i\in V_{bg}} \log(q_i)_{p_i}$$

- Laplacian loss (**for all pixels**)

$$\ell_{lp} = \frac{1}{2|V|}\sum_{i\in V}\sum_{j\in V} \Phi_{i,j}\left\|q_i - q_j\right\|_2^2,$$

$$\Phi_{i,j} = \begin{cases} \exp\left(-\frac{\left\|\bar{I}_i - \bar{I}_j\right\|^2}{2\sigma_1^2} - \frac{\left\|\bar{f}_i - \bar{f}_j\right\|^2}{2\sigma_2^2}\right) & \text{if } j \in N_i \\ 0 & \text{otherwise} \end{cases}$$

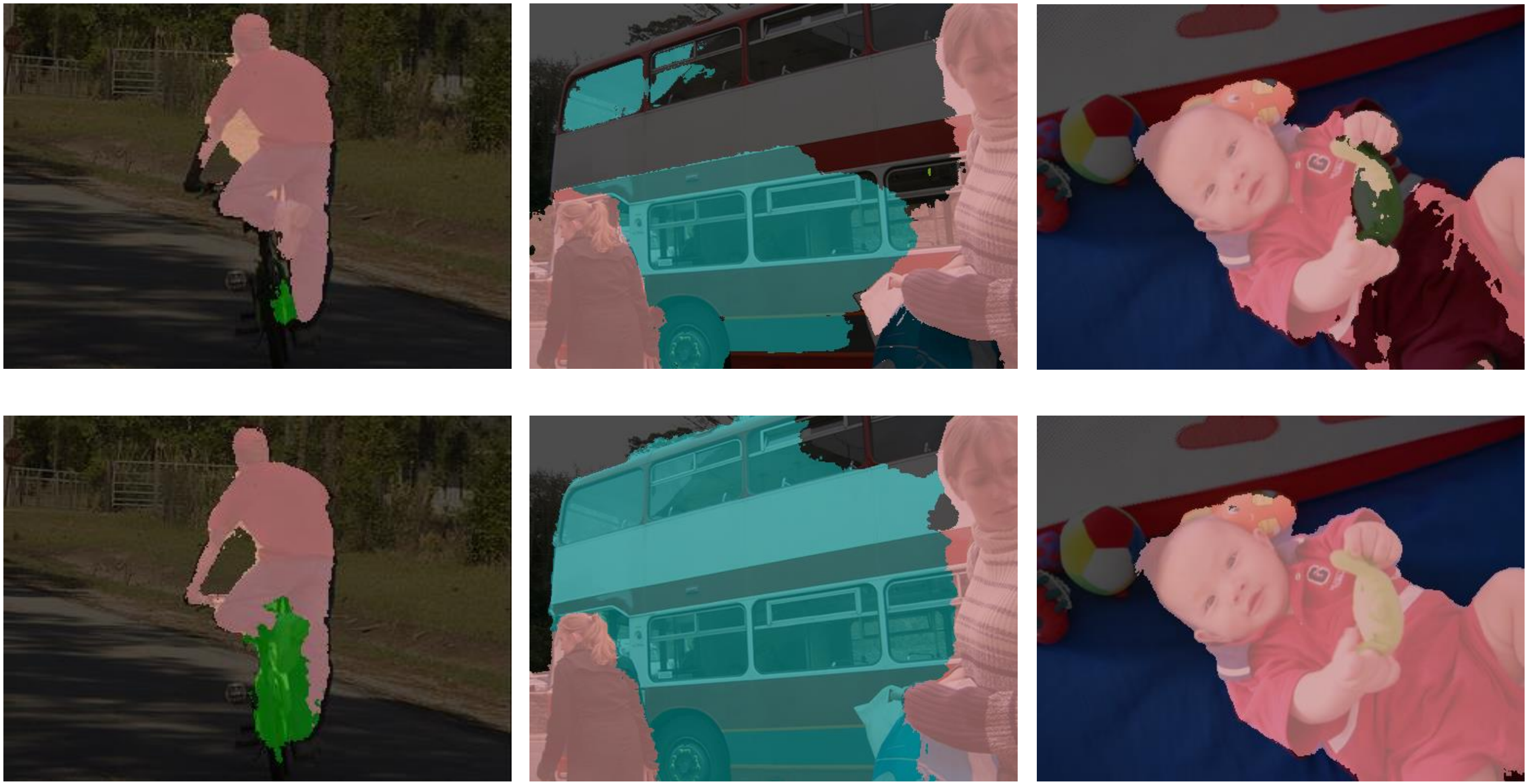
- Entropy loss (**for unlabeled pixels**)

$$\ell_{ent} = -\frac{1}{|V_{ig}|}\sum_{i\in V_{ig}}\sum_{c\in \bar{C}} (q_i)_c \log(q_i)_c$$

Results on PASCAL VOC 2012

IRNet
(Baseline)

WSGCN
(Ours)



Ahn et al., “Weakly supervised learning of instance segmentation with interpixel relations,” in CVPR, 2019.

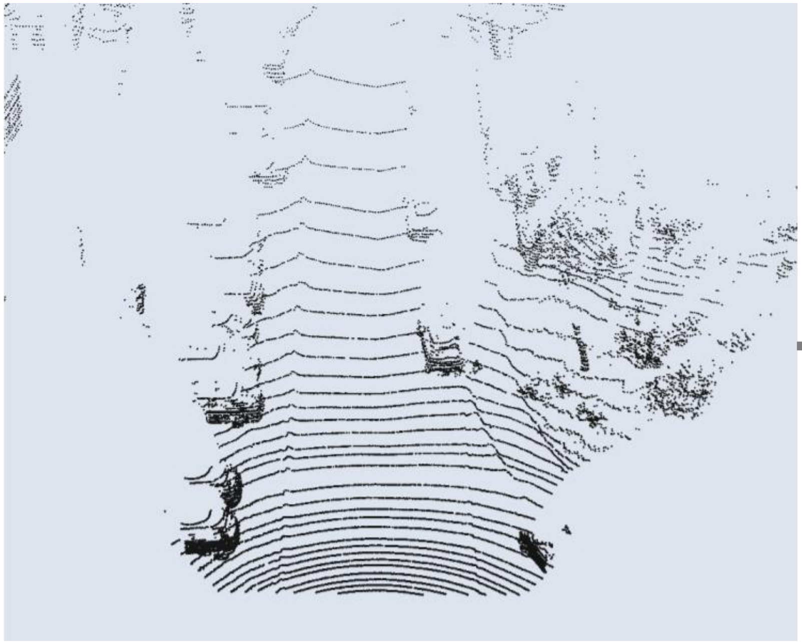
Point-GNN: Graph Neural Network for 3D Object Detection in a Point Cloud

Weijing Shi and Ragunathan (Raj) Rajkumar
Carnegie Mellon University

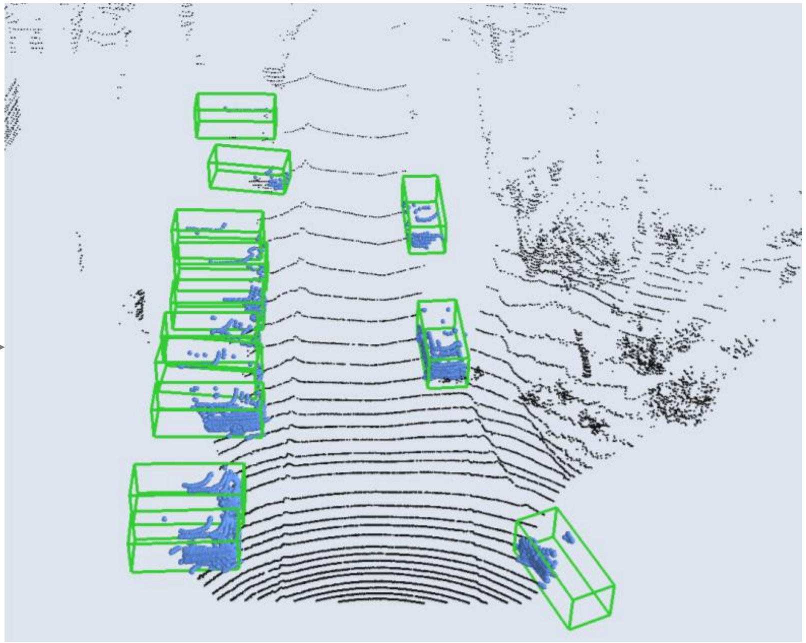
IEEE Conference on Computer Vision and Pattern Recognition (CVPR), 2020.

Task Specification

- To predict a 3D bounding box around group of 3D points representing 3 classes (car, pedestrian, cyclist)



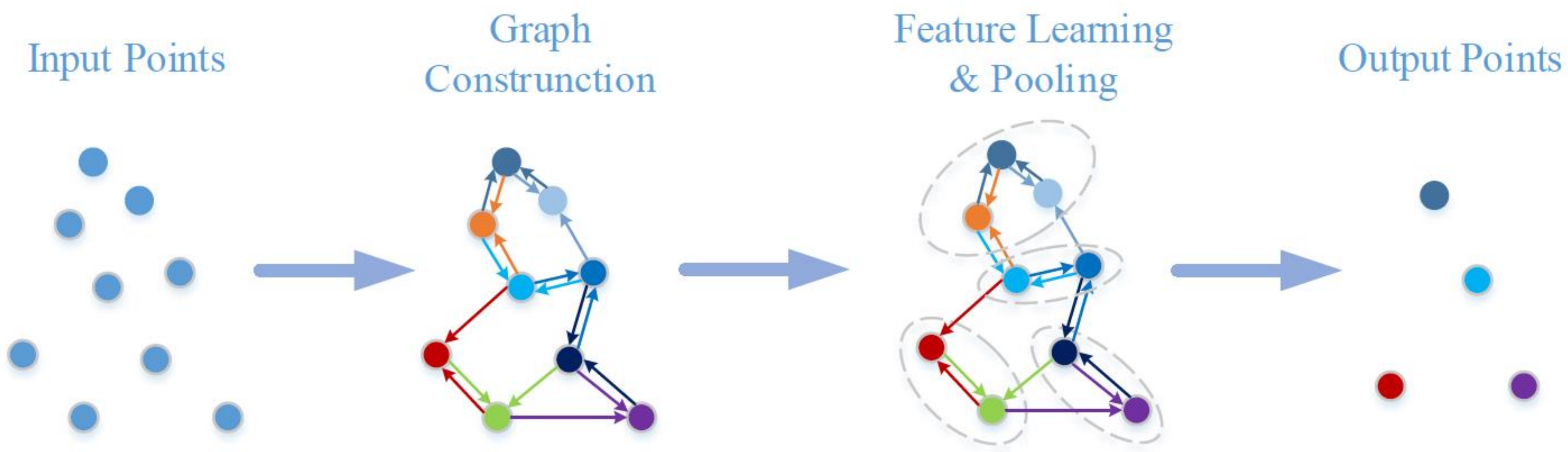
Input



Output
(only car class is shown)

GNN in 3D Point Cloud

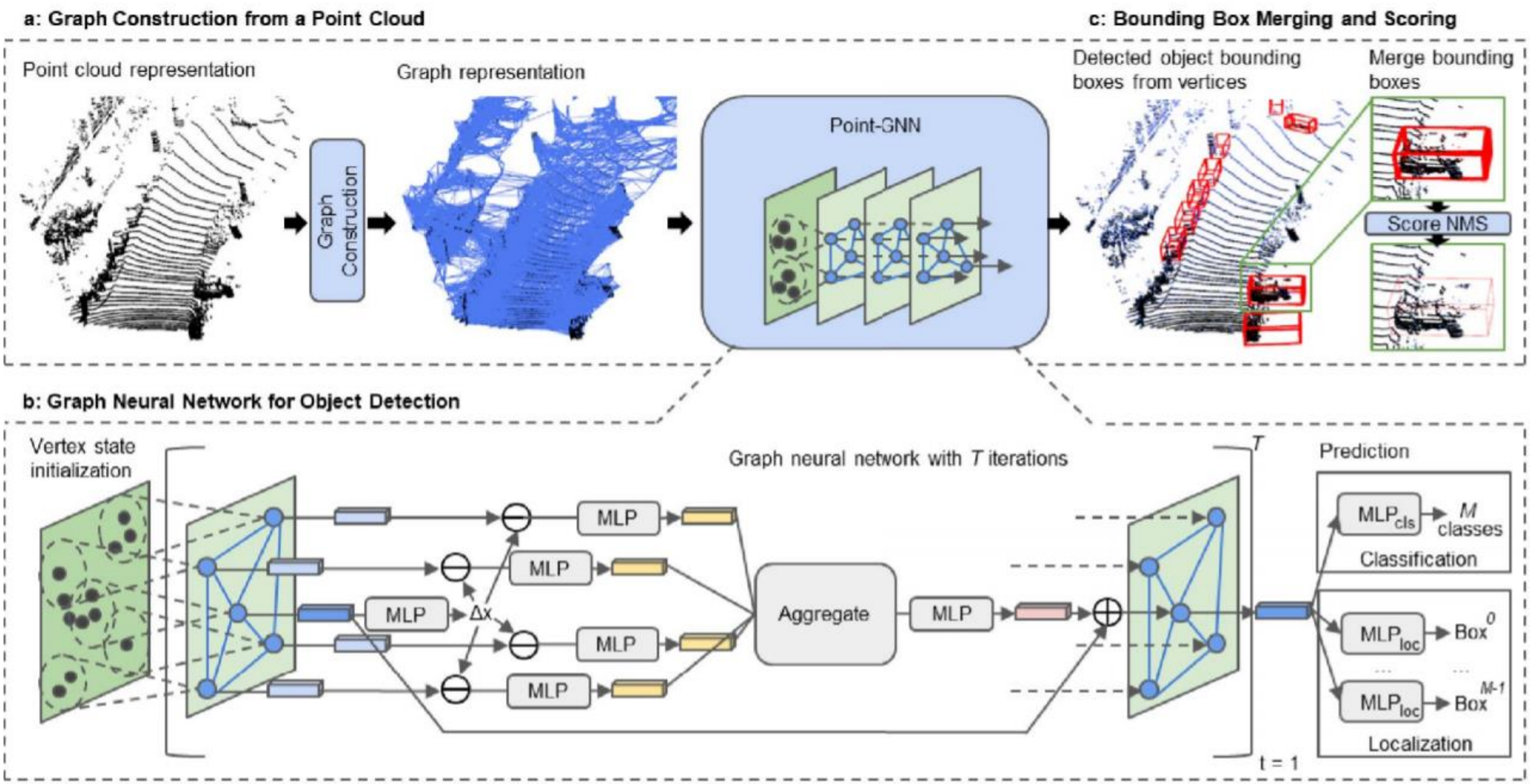
- Each point in a point cloud is a vertex of a graph
- Directed edges are formed for the graph
- Feature learning is performed in spatial domain



Guo et al., "Deep Learning for 3D Point Clouds: A Survey," IEEE TPAMI'20.

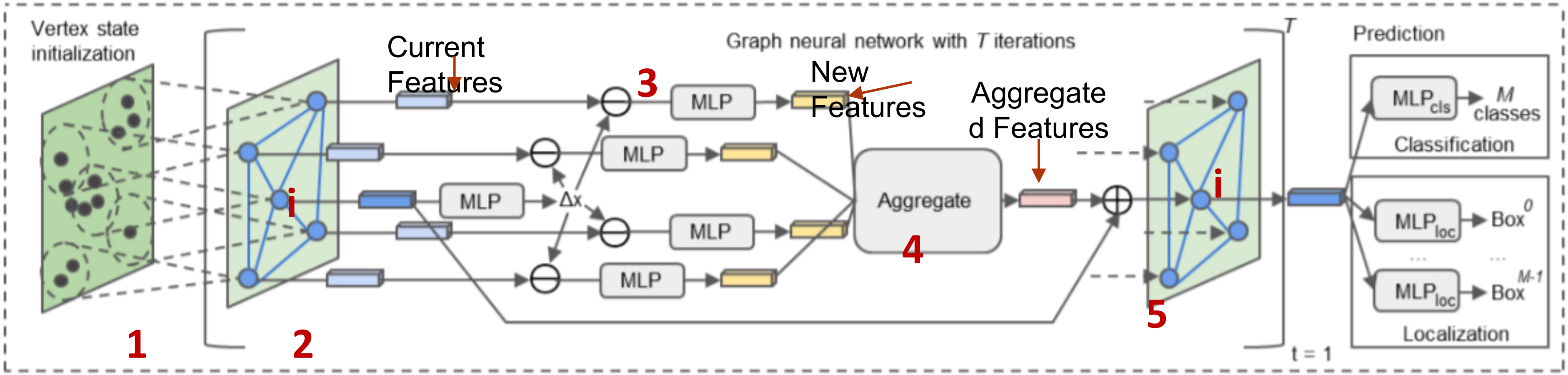
3D Object Detection in 3D Point Cloud

- Point-GNN



Shi et al., "Point-GNN: Graph Neural Network for 3D Object Detection in a Point Cloud ," in CVPR, 2020.

3D Object Detection in 3D Point Cloud



1. Point Cloud down-sampling to reduce initial point cloud size

2. Graph formation by connecting a point to its neighbors within a fixed radius r.

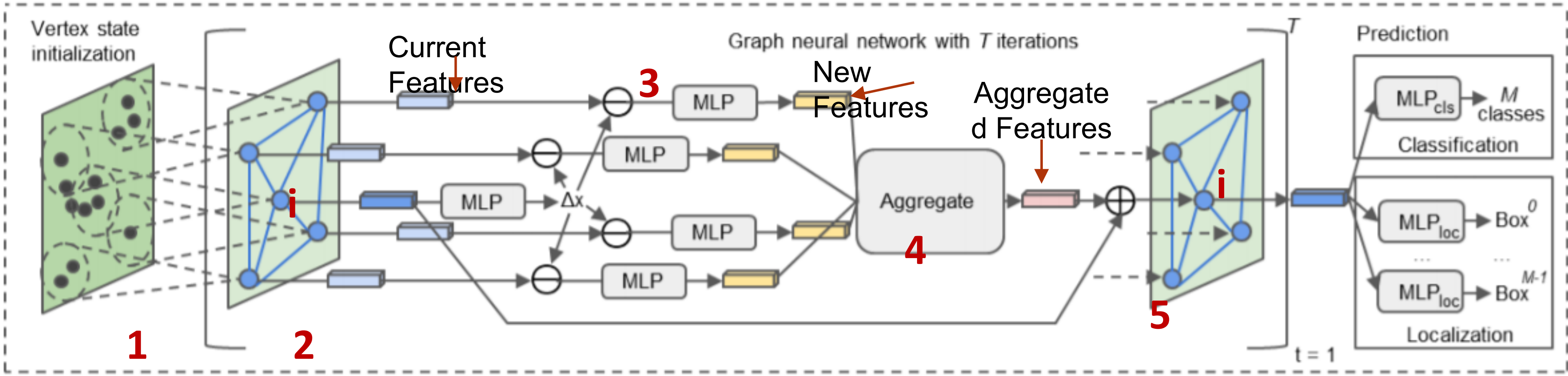
$$Graph\ G = (P, E)$$

P = Vertices = points in point cloud

E = Edges = $\left\{(p_i, p_j) \middle| \left\|x_i - x_j\right\|_2 < r\right\}$

Shi et al., “Point-GNN: Graph Neural Network for 3D Object Detection in a Point Cloud ,” in CVPR, 2020.

3D Object Detection in 3D Point Cloud



3. Each neighborhood vertex's MLP's input is its current features and an offset generated by MLP of the center vertex i. The output is learned new features

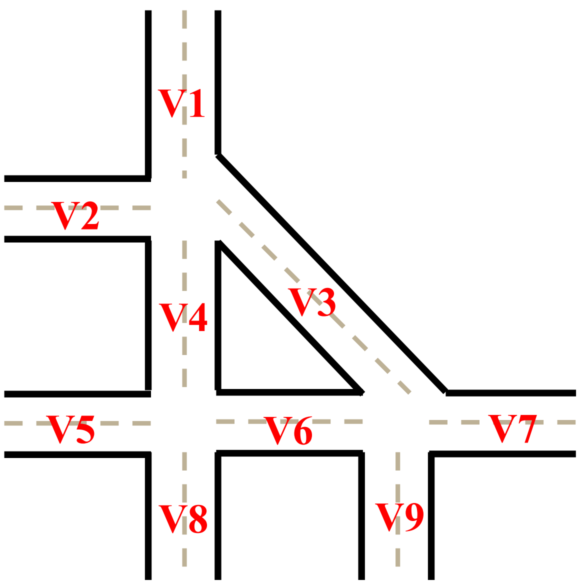
4. Feature aggregation stage aggregates new features of neighboring vertices and produce new aggregated features for center vertex i. Aggregated features become new current features of center point

5. Graph is updated with new features for each vertex. The loop follows until specific iterations T

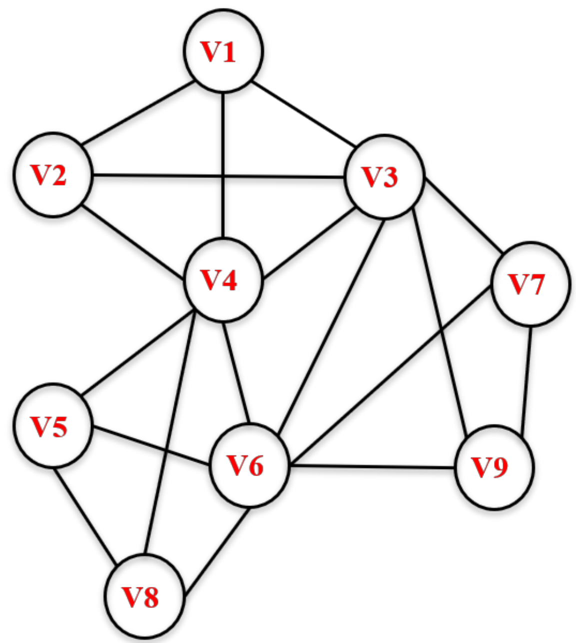
Shi et al., "Point-GNN: Graph Neural Network for 3D Object Detection in a Point Cloud ," in CVPR, 2020.

Traffic Prediction Using STGNN

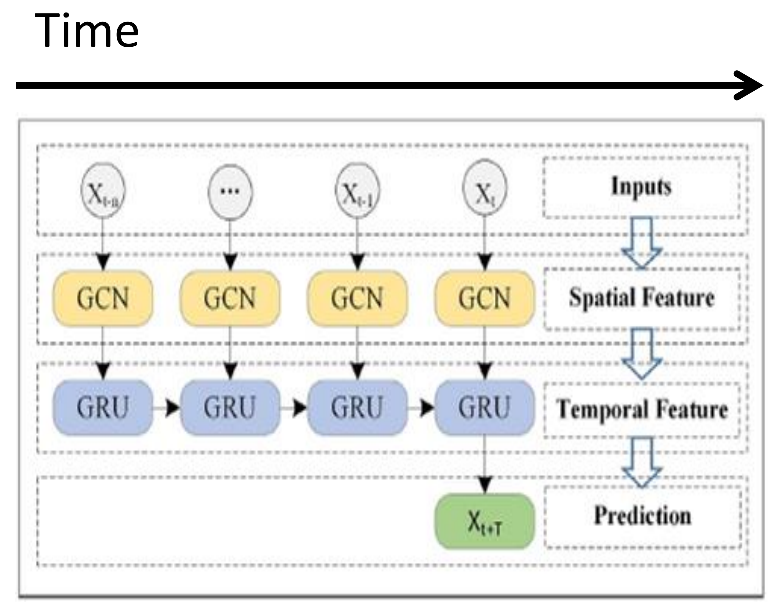
- To predict traffic conditions on urban roads based on time-series data



Map



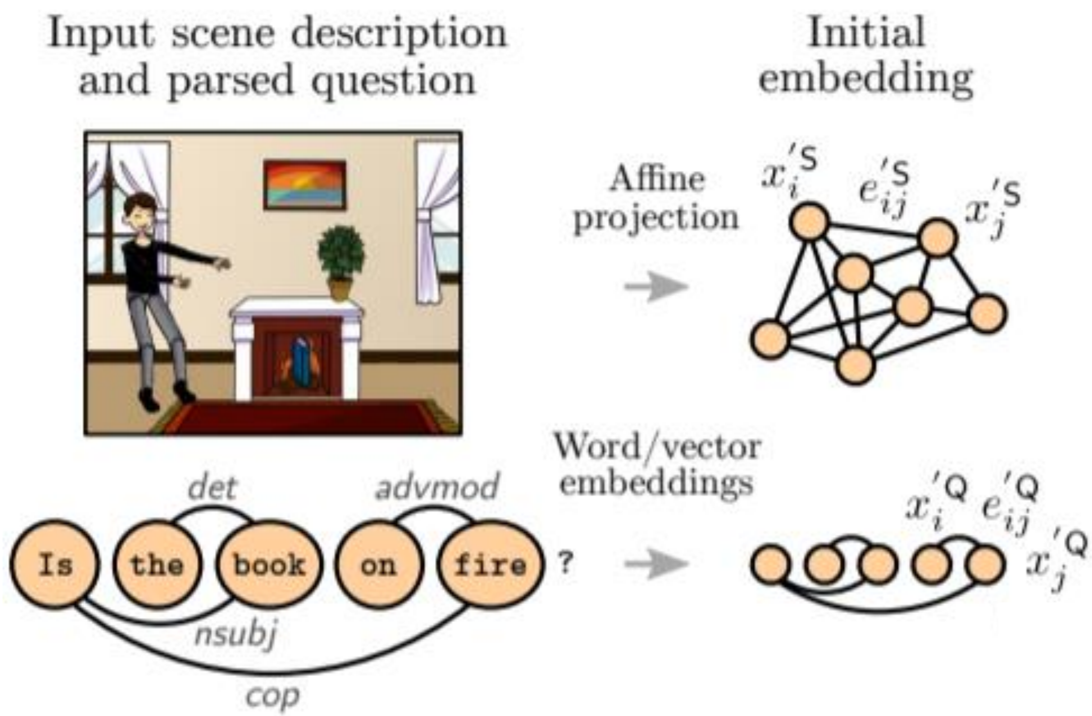
Graph Topology



STGCNN

Visual Question Answering

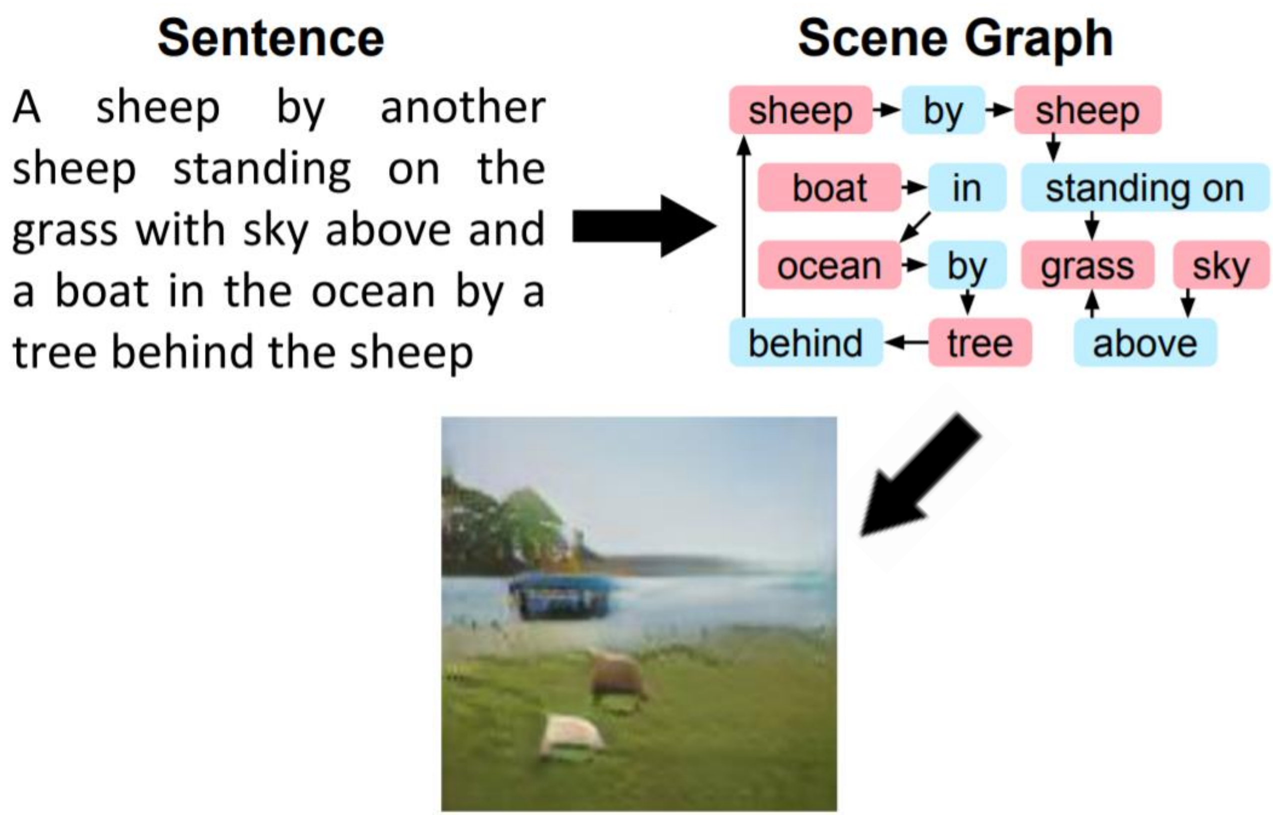
- To answer questions based on description of an image
- Encode the descriptions of scene and question as graphs
- Scene – **node**: objects; **edge**: spatial arrangement
- Question – **node**: words; **edge**: syntactic dependencies



Teney et al., "Graph-structured representations for visual question answering," in CVPR'17

Text to Image Synthesis

- To generate images from natural language descriptions
- Convert sentences to scene graphs
- Generate images from scene graphs



J. Johnson et al., “Image generation from scene graphs,” CVPR’18

Thank you for your attention

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- Shi et al., “Point-GNN: Graph Neural Network for 3D Object Detection in a Point Cloud ,” in CVPR, 2020.