



CSCI587 – Lecture 18

Spatiotemporal Forecasting

10/30/2024

*University of Southern California
USC Viterbi School of Engineering
Fall 2024*



Introduction – Spatiotemporal Data

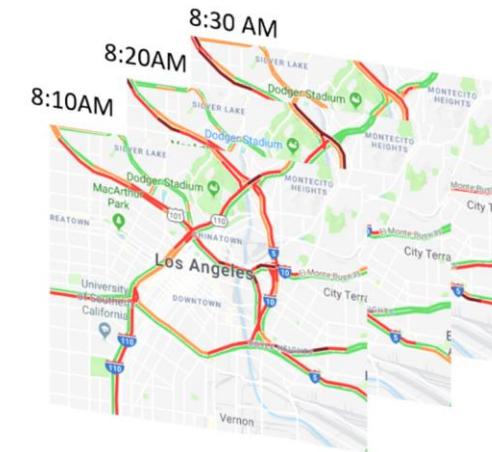
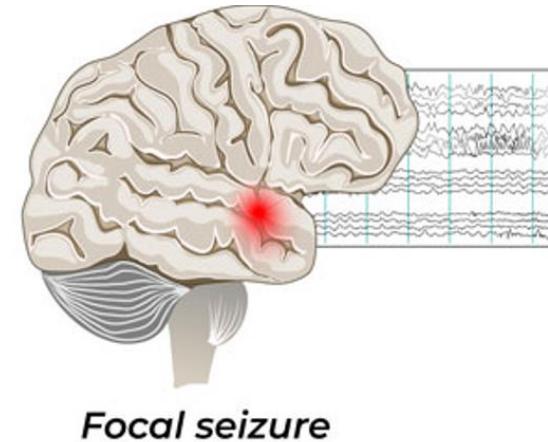
- **Spatiotemporal Data:** Where + When
- **Unique Characteristics**
 - Massive amounts of high-frequency data from numerous locations
 - Rich underlying patterns across both space and time
- **Why it matters?**
 - Critical for decision making in many domains, e.g., urban planning





Introduction – Spatiotemporal Forecasting

- **Spatiotemporal Forecasting:** Predict events or conditions in space & time by analyzing spatiotemporal data
- **Examples**
 - **POI Visit Forecasting:** Predicting the # of visits to specific POIs at different times
 - **Seizure Detection:** Predicting the occurrence of seizures in specific brain regions during particular time intervals.
 - **Traffic Forecasting:** Predicting traffic flow on roads during various times of day





You've already learned about **Spatial** data...

*...but what is the **Temporal** dimension?*



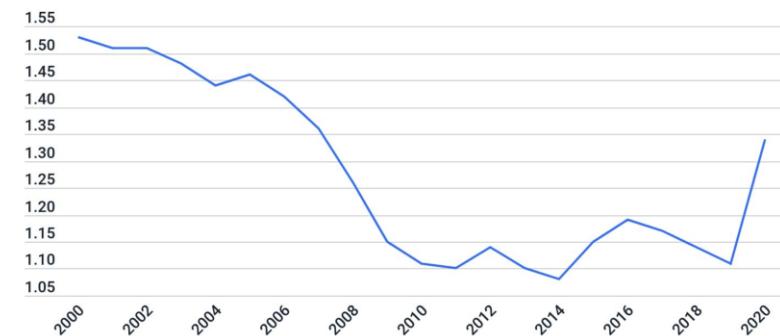
Time Series

Time series

A **sequence** of observations collected over time.

$$x_i = (x_{i1}, x_{i2}, \dots, x_{iT}) \in \mathbb{R}^T$$

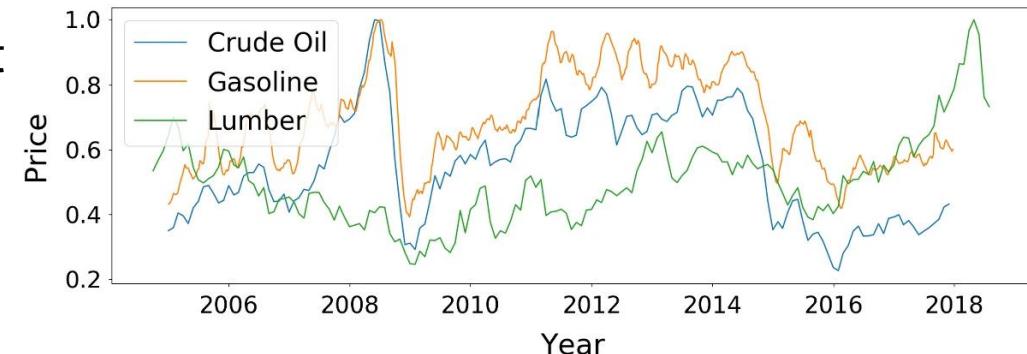
Car Crash Fatality Rate Per 100 Million Miles Traveled



Multivariate Time series

A **collection** of two or more **time series** observed over time, with each **variable** being **dependent** on its own past values as well as the past values of the other series.

$$X = (x_1, x_2, \dots, x_N) \in \mathbb{R}^{N \times T}$$





Time Series Forecasting

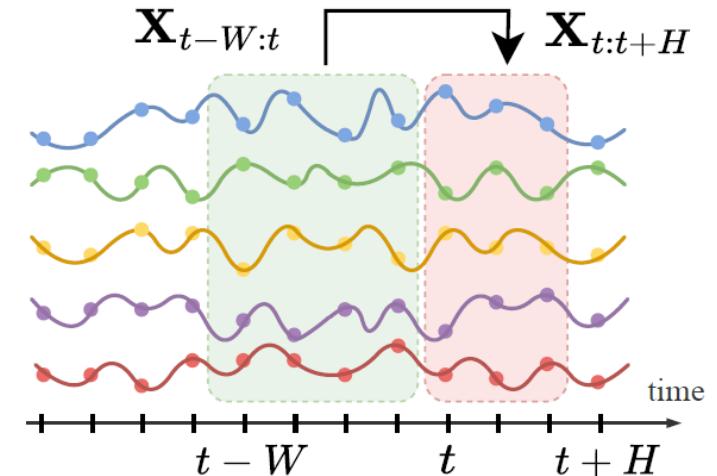
Time Series Forecasting

Given a window of $W \geq 1$ of **past** observations:

$$X_{t-W:t} = [X_{t-W}, \dots, X_{t-1}],$$

Predict $H \geq 1$ **future** observations:

$$X_{t:t+H} = [X_t, \dots, X_{t+H-1}]$$



Thus, the goal is to learn a **model** F with parameters θ that maps past observations to future values:

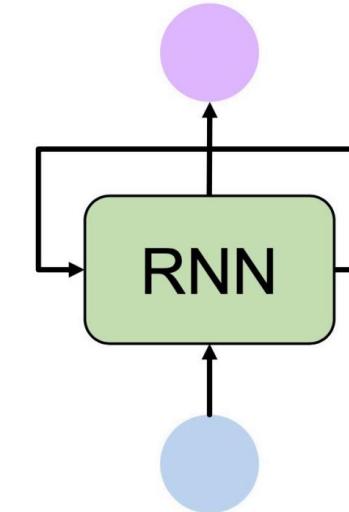
$$F(X_{t-W:t}, \theta) = X_{t:t+H}$$

Sequence Modeling



To model **sequences**, we need to:

- Handle **variable-length** sequences
- Track **long-term** dependencies
- Maintain information about **order**
- **Share** parameters across the sequence

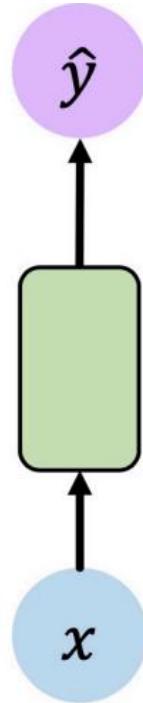


Popular solution:

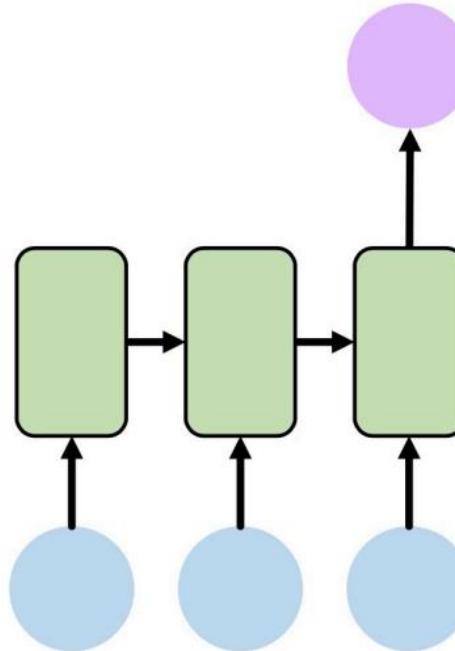
- Recurrent Neural Networks (**RNNs**)



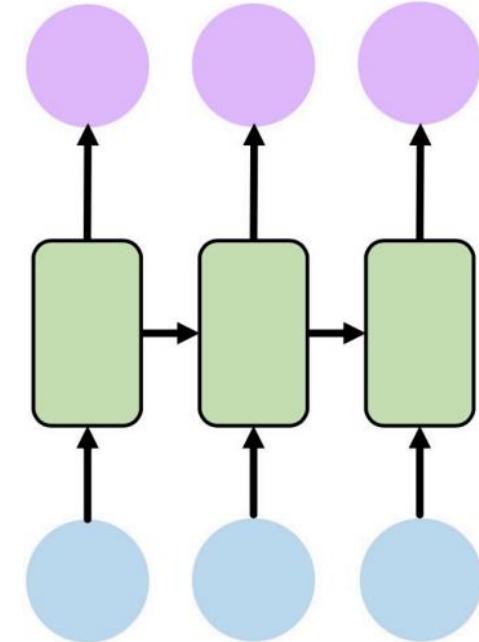
Recurrent Neural Networks



One to One
“Vanilla” Neural Network



Many to One
E.g., Sentiment Classification



Many to Many
E.g., Music Generation

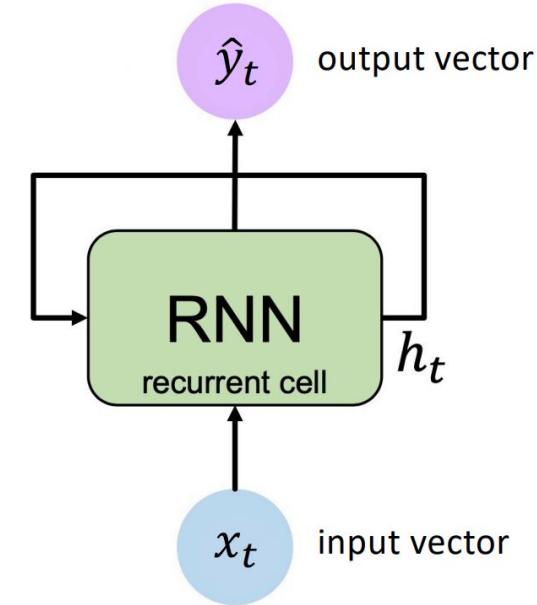


A Recurrent Neural Network (RNN)

- Apply a recurrence relation at every time step to process a sequence:

cell state old state
$$h_t = f_W(h_{t-1}, x_t)$$

A function current
parameterized input
by W

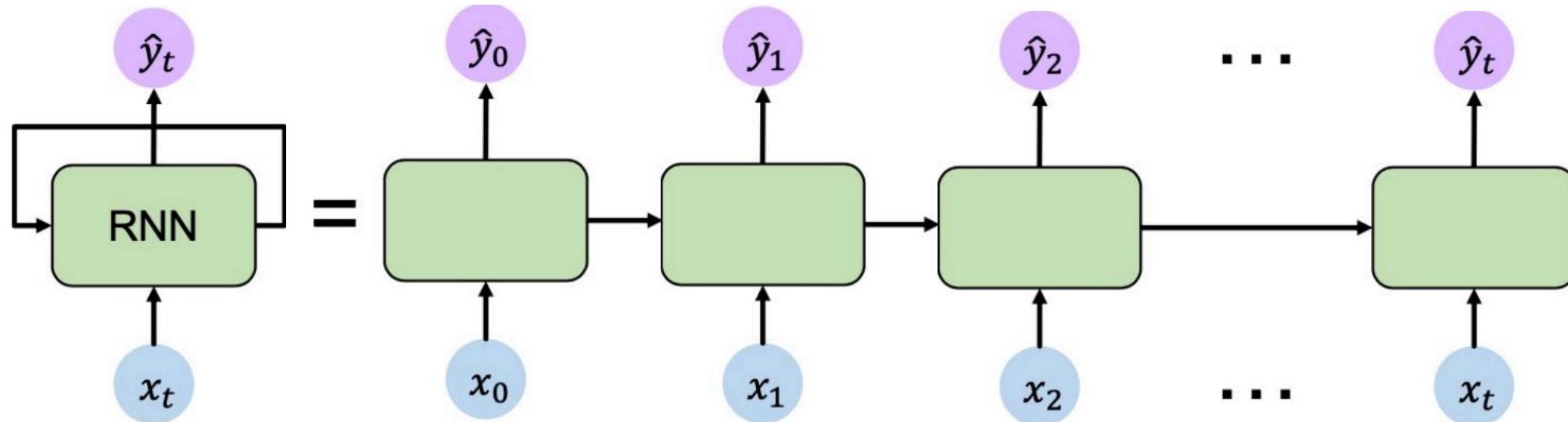


Note: The **same function** and **set of parameters** are used at every time step.

RNN – Computational Graph Across Time



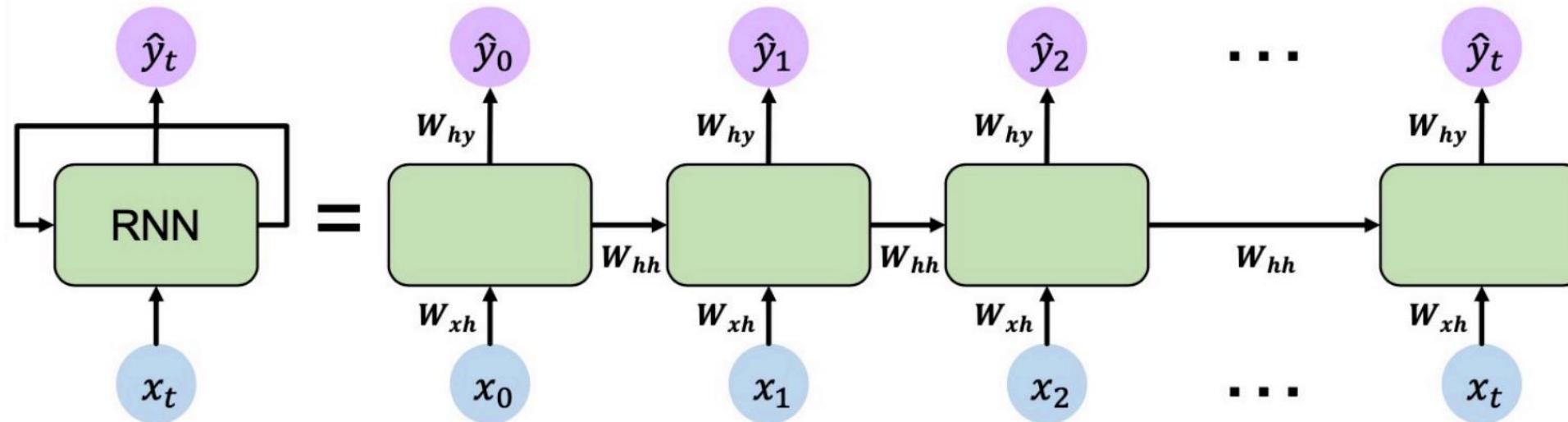
- Represent as computational graph **unrolled** over time





RNN – Computational Graph Across Time

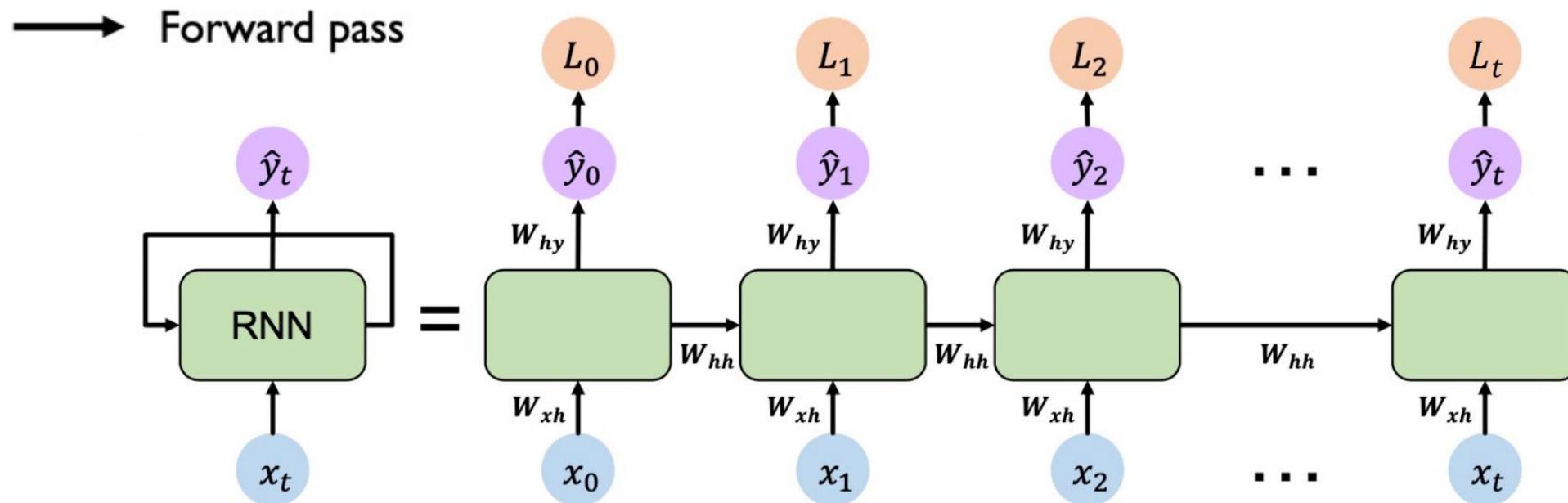
- Re-use the **same weight matrices** at every time step





RNN – Computational Graph Across Time

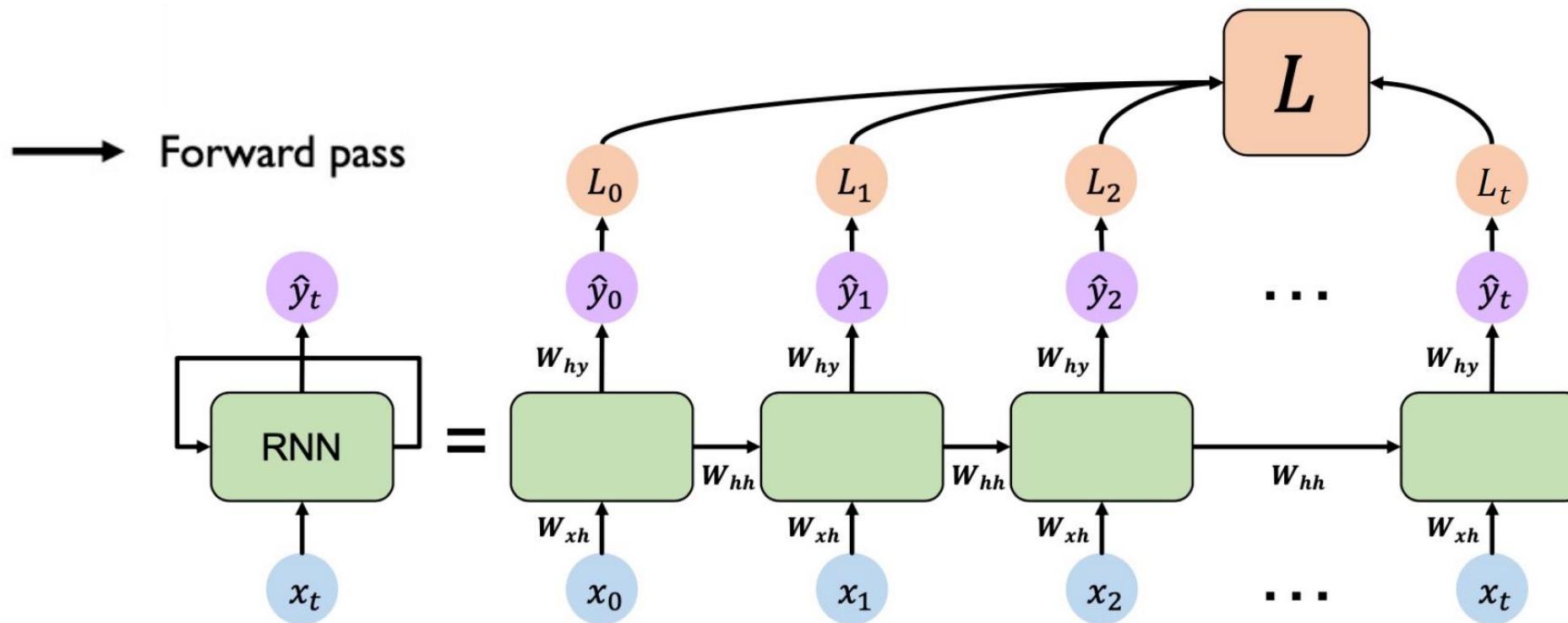
- Compute the loss L_t by comparing \hat{y}_t and y_t (y_t is ground truth)
 - E.g., $L_t = (\hat{y}_t - y_t)^2$





RNN – Computational Graph Across Time

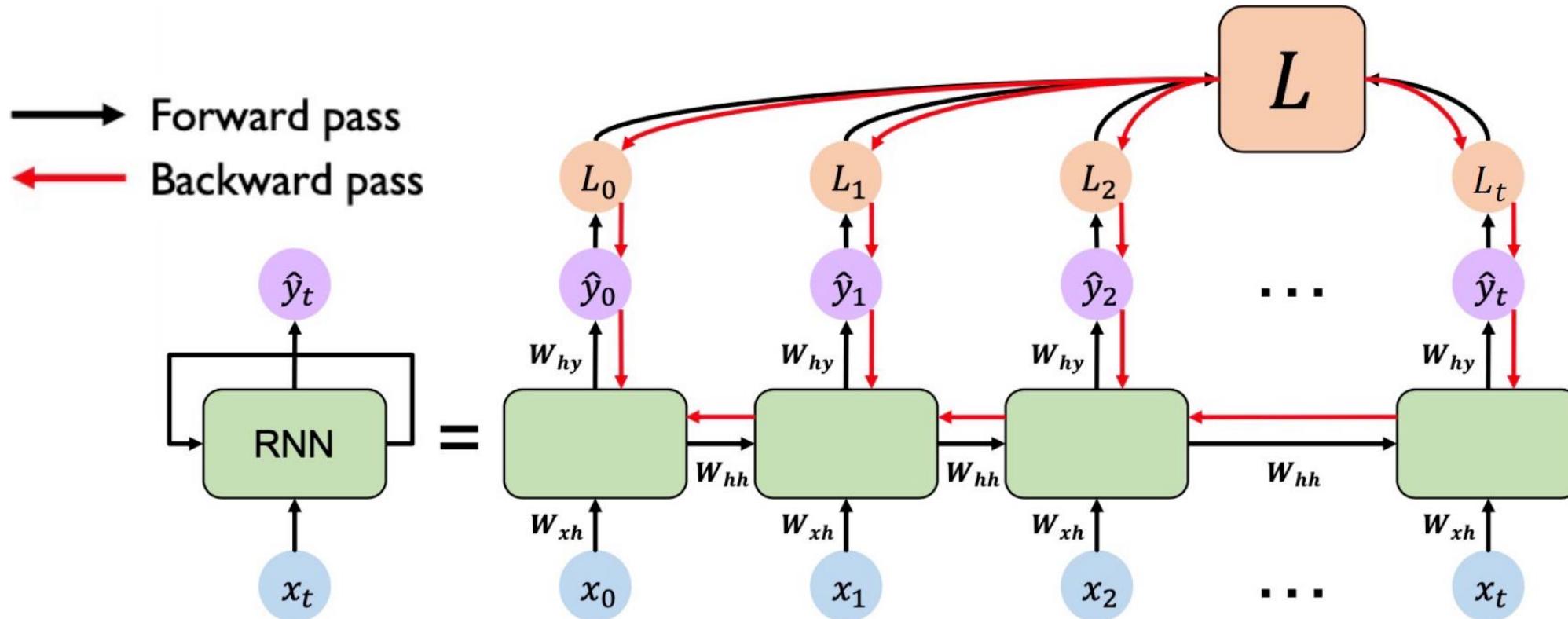
- Total Loss: $L = \sum_{t=1}^T L_t$



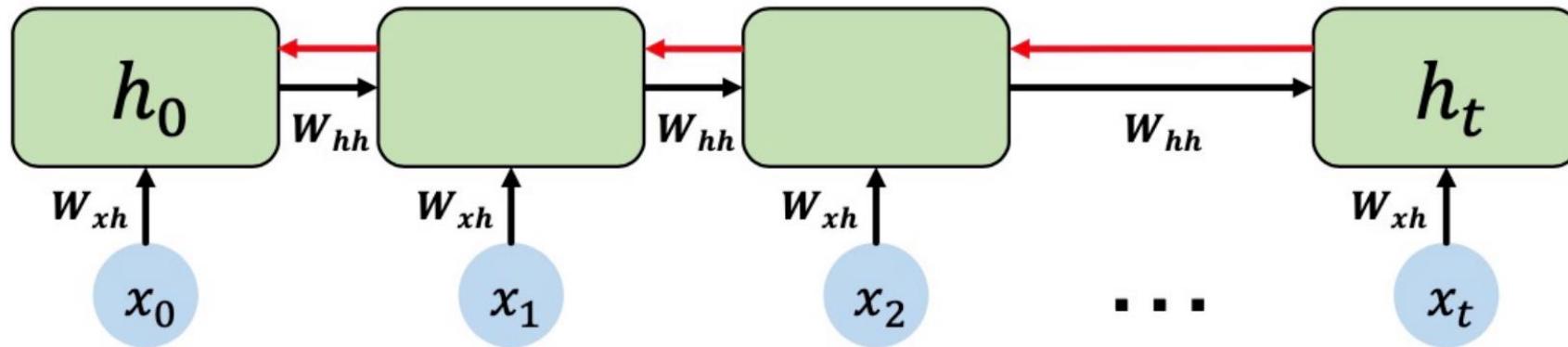
RNN – Backpropagation Through Time



- For backpropagation, we need to compute the gradients w.r.t. W_{hy}, W_{hh}, W_{xh}



RNN – Backpropagation Through Time



Computing the gradient involves **many multiplications** (and repeated f')

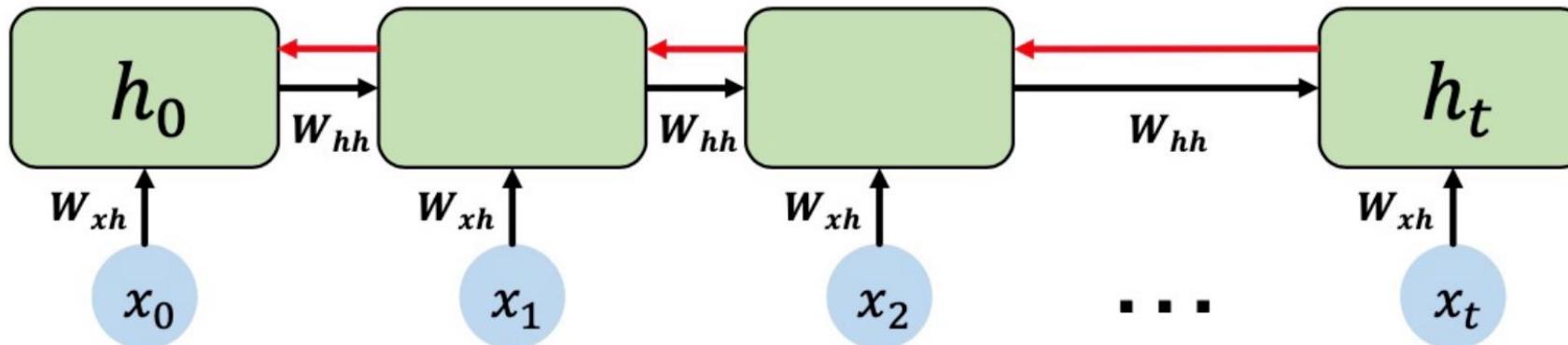
- When w_{hh} changes (in a small amount), how much would L change?

For example,

$$\frac{\partial L}{\partial w_{hh}} = \frac{1}{T} \sum_{t=1}^T \frac{\partial l(y_t, \hat{y}_t)}{\partial w_{hh}}$$
$$h_t = \tanh(\mathbf{W}_{xh}x_t + \mathbf{W}_{hh}h_{t-1})$$
$$= \frac{1}{T} \sum_{t=1}^T \frac{\partial l(y_t, \hat{y}_t)}{\partial \hat{y}_t} \frac{\partial g(h_t, w_{hy})}{\partial h_t} \boxed{\frac{\partial h_t}{\partial w_{hh}}} \quad \frac{\partial h_t}{\partial w_{hh}} = \frac{\partial f(x_t, h_{t-1}, w_{hh})}{\partial w_{hh}} = \frac{\partial f(x_t, h_{t-1}, w_{hh})}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial w_{hh}}.$$



RNNs – Gradient Flow Issues



Computing the gradient involves **many multiplications** (and repeated f')

Case 1: Many values are > 1

Exploding gradients

Trick : Gradient clipping to scale big gradients

Case 2: Many values are < 1

Vanishing gradients

Trick 1: Activation functions
Trick 2: Network architecture

Remedy to the Gradient Flow Issues



- Use a more complex recurrent unit with **gates** to **control what information is passed through**

gated cell

LSTM, GRU, etc.

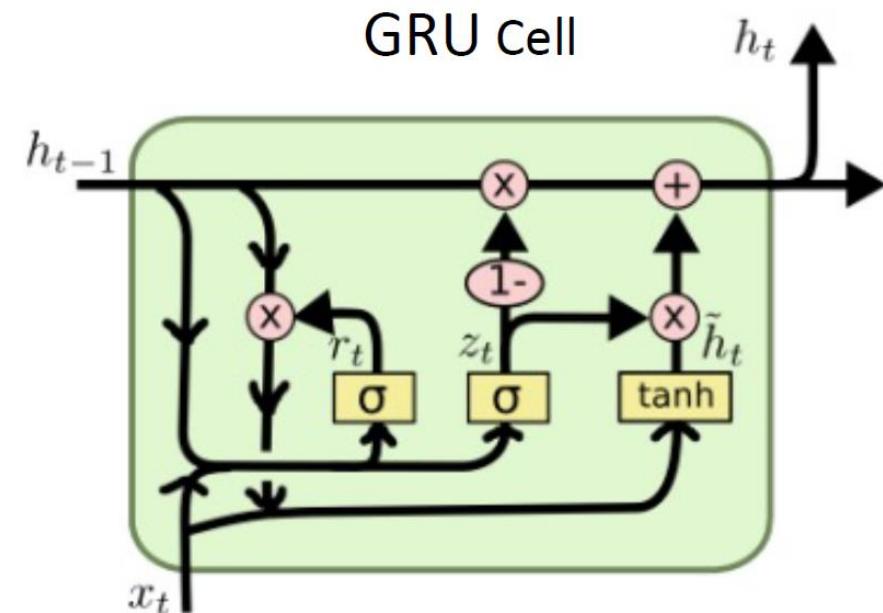
- **Long Short-Term Memory (LSTM)** and **Gated Recurrent Unit (GRU)** networks rely on gated cells to track information throughout many time steps.



Gated Recurrent Unit (GRU)

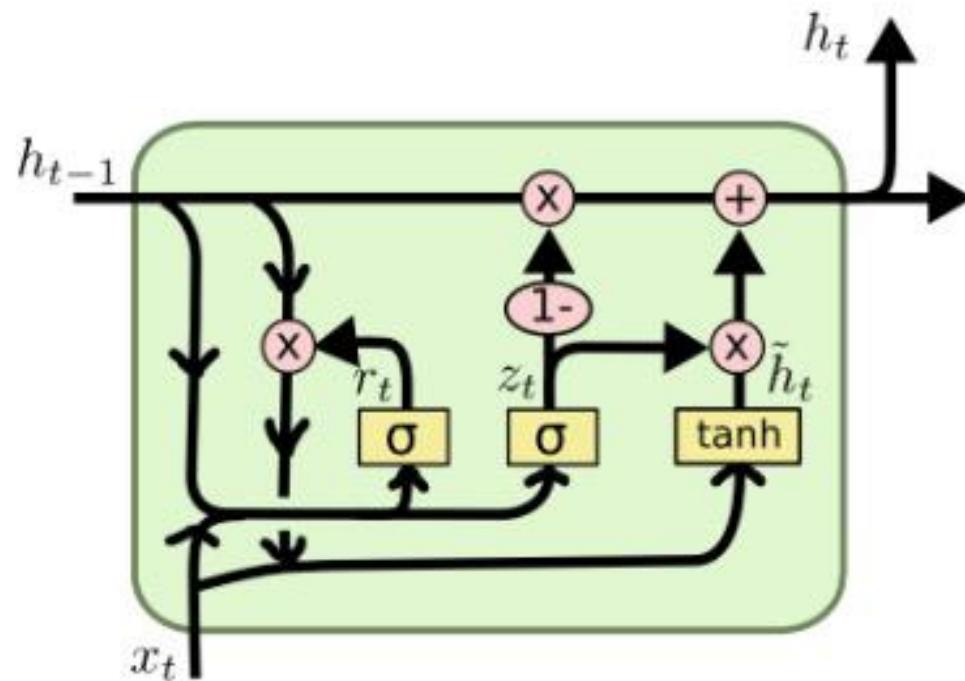
- GRU is an RNN variant with **gating** mechanisms to control **information flow**, helping to prevent **vanishing gradients**.

$$z_t = \sigma(W_z[h_{t-1}, x_t] + b_z)$$
$$r_t = \sigma(W_r[h_{t-1}, x_t] + b_r)$$
$$\tilde{h}_t = \tanh(W_h[r_t \odot h_{t-1}, x_t] + b_h)$$
$$h_t = z_t \odot h_{t-1} + (1 - z_t) * \tilde{h}_t$$





GRU – Update Gate

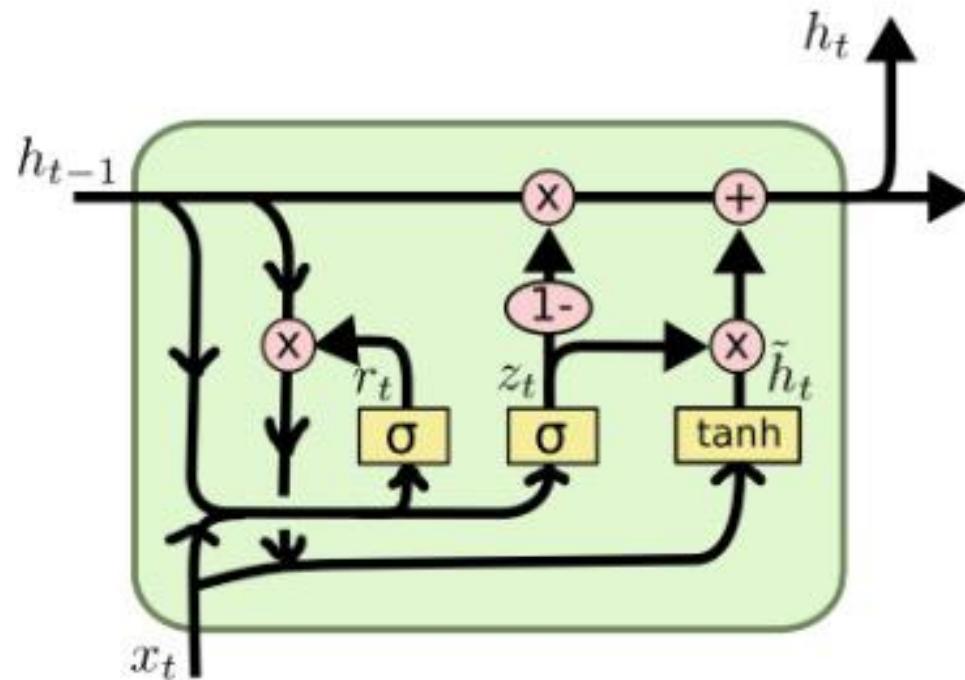


$$z_t = \sigma(W_z[h_{t-1}, x_t] + b_z)$$

- Concatenate previous hidden state and current input
- Update gate controls what parts of hidden state are **updated** (used as z_t) vs. **preserved** (used as $(1 - z_t)$)



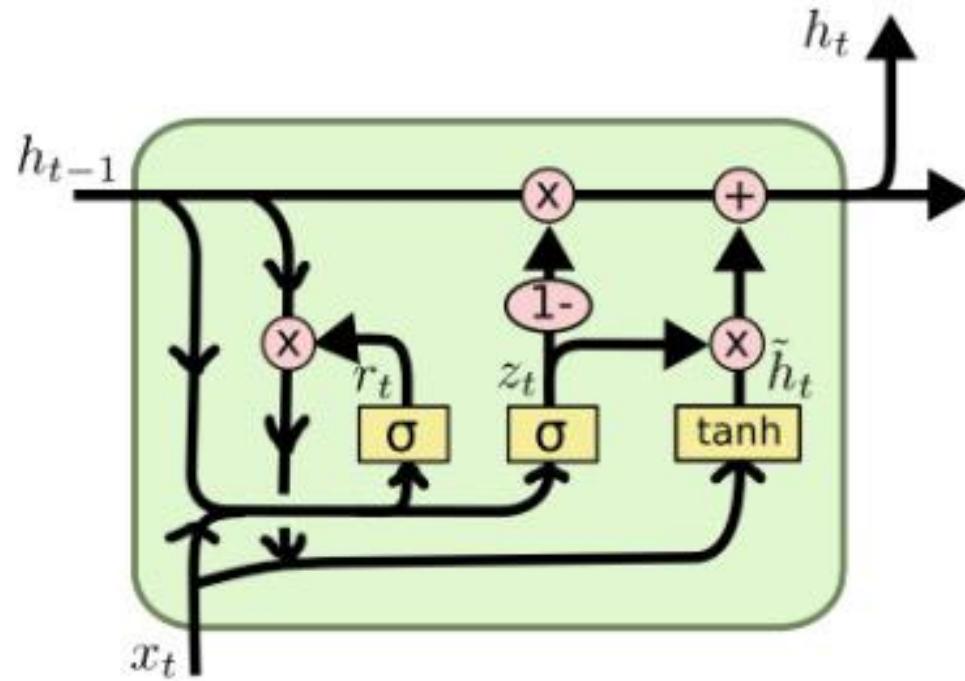
GRU – Reset Gate



$$r_t = \sigma(W_r[h_{t-1}, x_t] + b_r)$$

- Reset gate controls what parts of **previous hidden state** are used to compute new content

GRU – New Hidden State Content

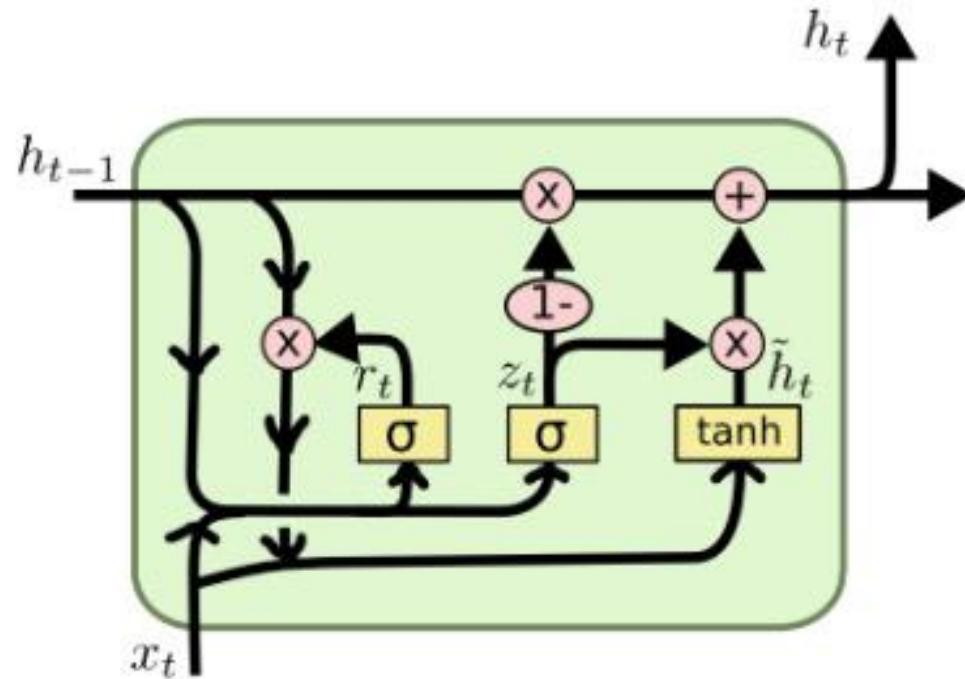


$$\tilde{h}_t = \tanh(W_h[r_t \odot h_{t-1}, x_t] + b_h)$$

- r_t selects useful parts of **previous hidden state**
- Use $r_t \odot h_{t-1}$ and **current input** to compute new hidden content



GRU – Output Hidden State



$$h_t = z_t \odot h_{t-1} + (1 - z_t) * \tilde{h}_t$$

- Update gate simultaneously controls what is **kept from previous hidden state**, and what is **updated to new hidden state content**



...Let's get back into the spatiotemporal tasks

Spatiotemporal Application: Traffic Forecasting Task



⋮



⋮



GIVEN: traffic measurements (e.g., avg speed of passing cars) over 12 timesteps of some road segments.

GOAL: Predict traffic measurements for the next 12 timesteps.



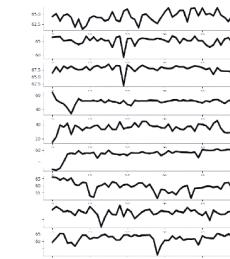
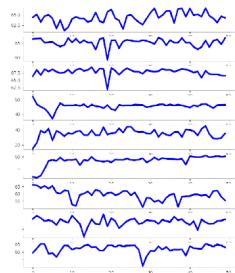
⋮



⋮

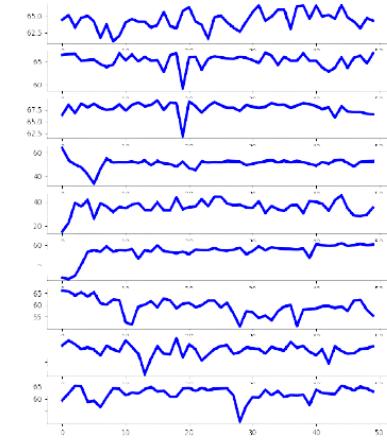


Traffic Prediction

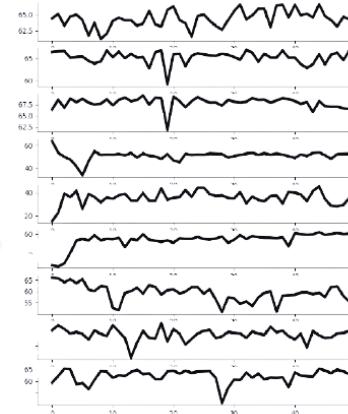
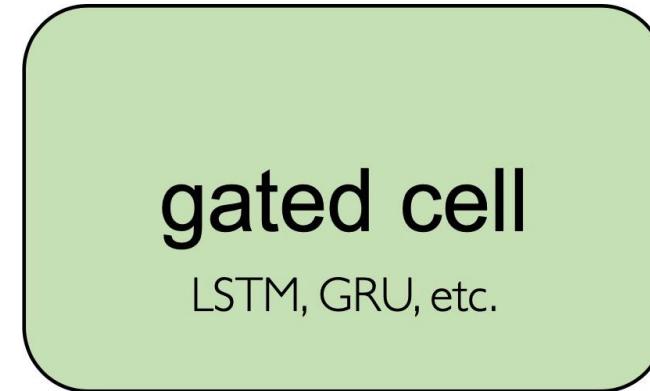




RNNs for Traffic Forecasting Task



Traffic Observations



Traffic Predictions

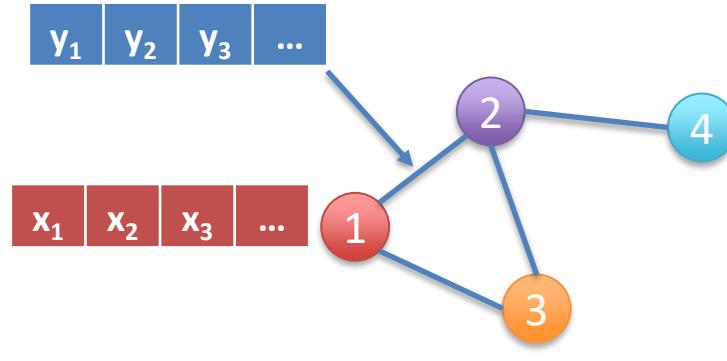
- **Straightforward Approach:** Pass the sequences to an RNN-based model to forecast future values.
- **What's wrong with this approach?**
 - **Missed inductive bias:** This ignores **spatial dependencies**, treating each location **independently** instead of leveraging the **connected road network structure**.



*To accurately model spatiotemporal tasks, we need an approach that leverages **the inductive bias of both spatial and temporal patterns** inherent in data, such as in road networks.*

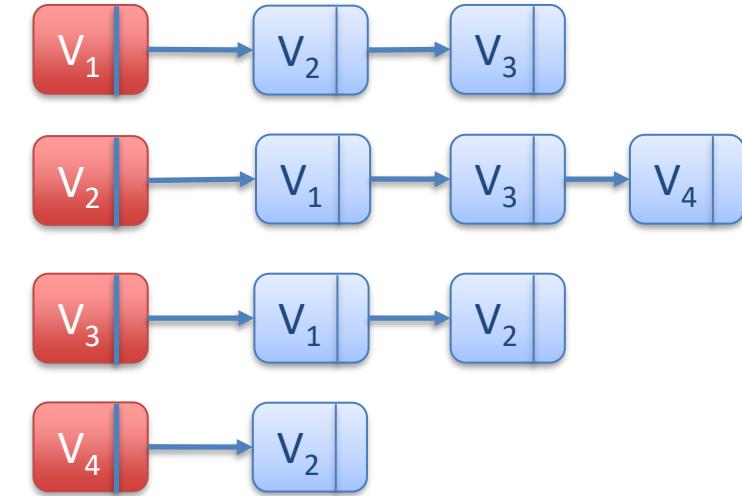


Graphs



	v_1	v_2	v_3	v_4
v_1	0	1	1	0
v_2	1	0	1	1
v_3	1	1	0	0
v_4	0	1	0	0

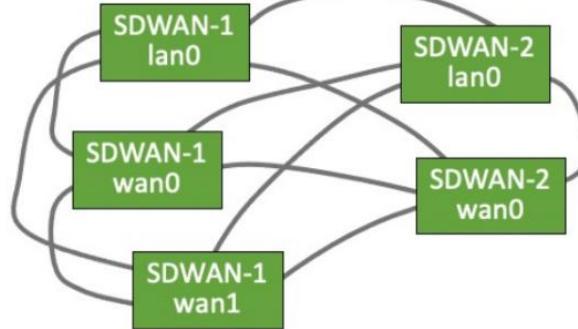
Adjacency Matrix
 $V \times V$



Modeling Real World Problems as Graphs



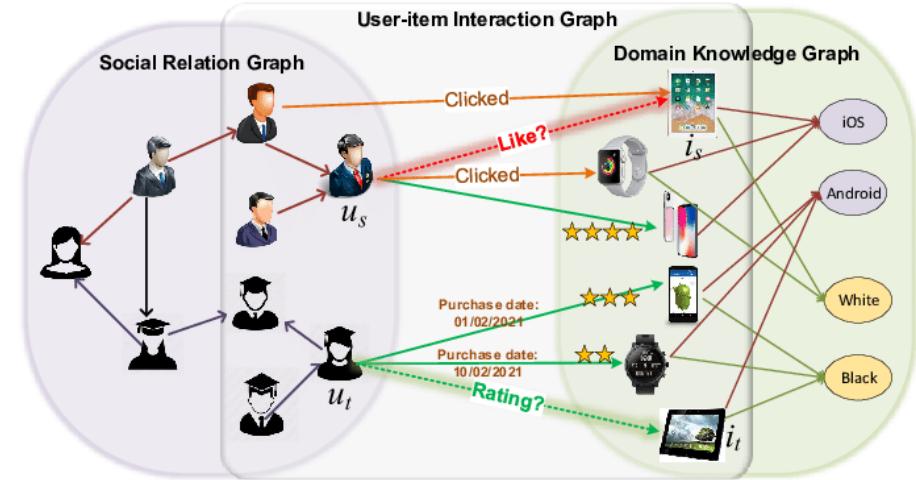
Road Network
(Veličković, 2021)



Computer Network Topology
(Lin, 2021)



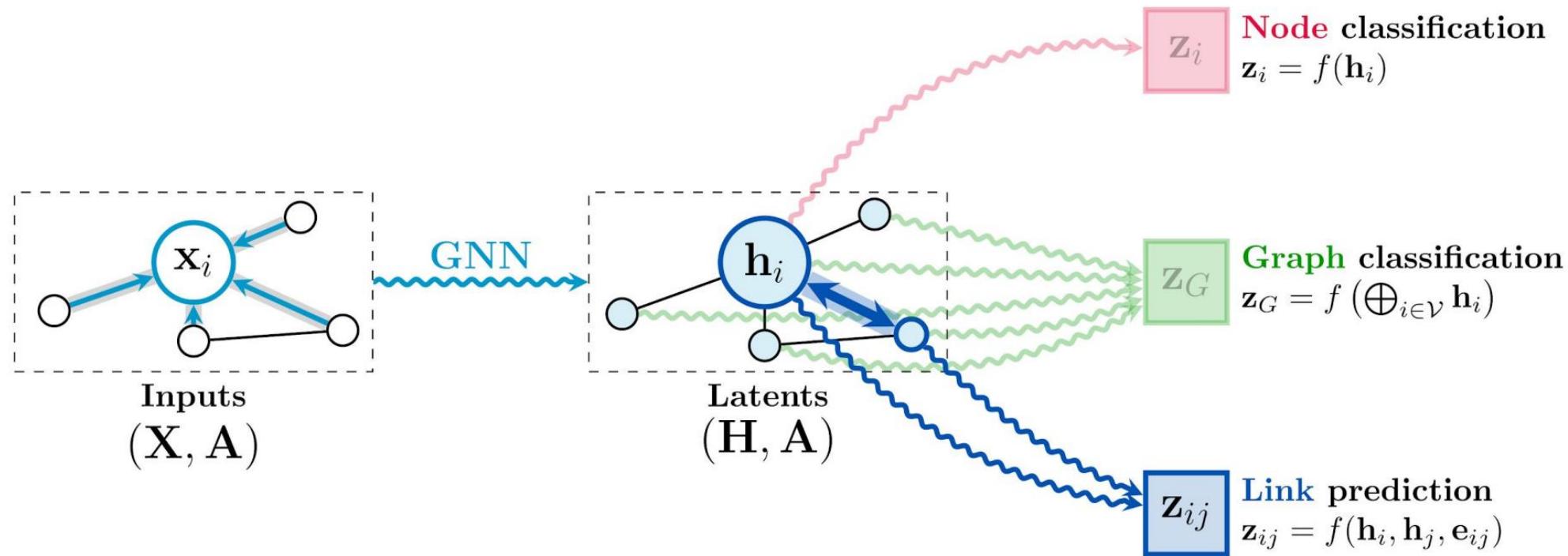
Social Networks



Recommendation Systems
(Wang, 2021)



Graph Neural Networks

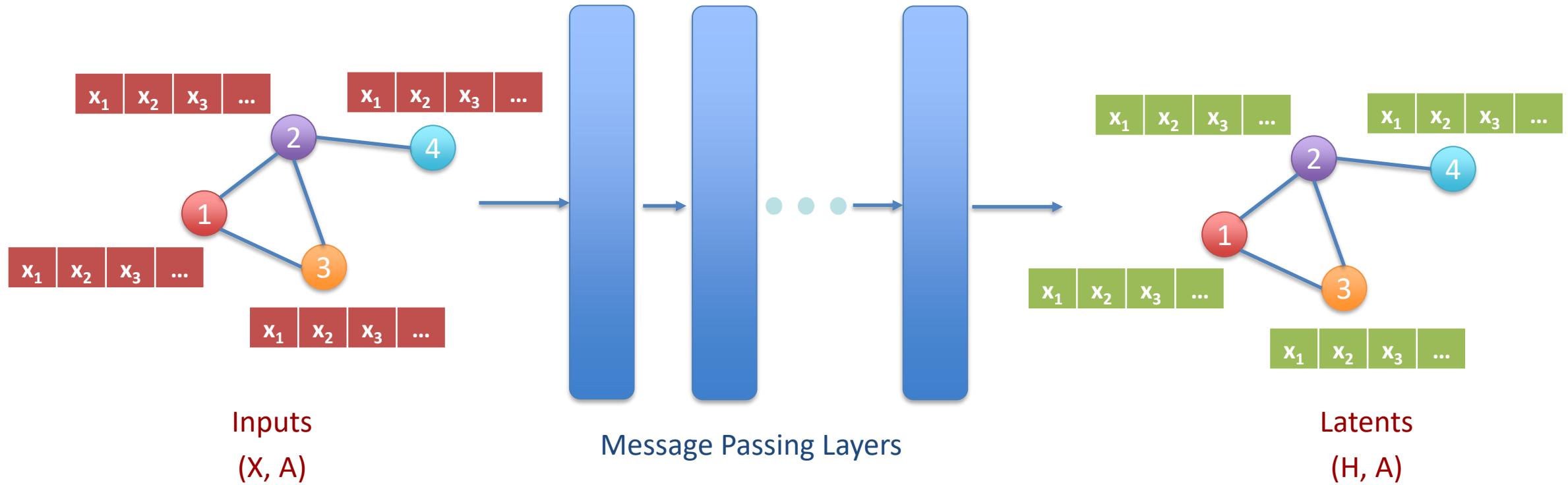


Using GNNs to Solve Machine Learning Problems

(Veličković, 2021)



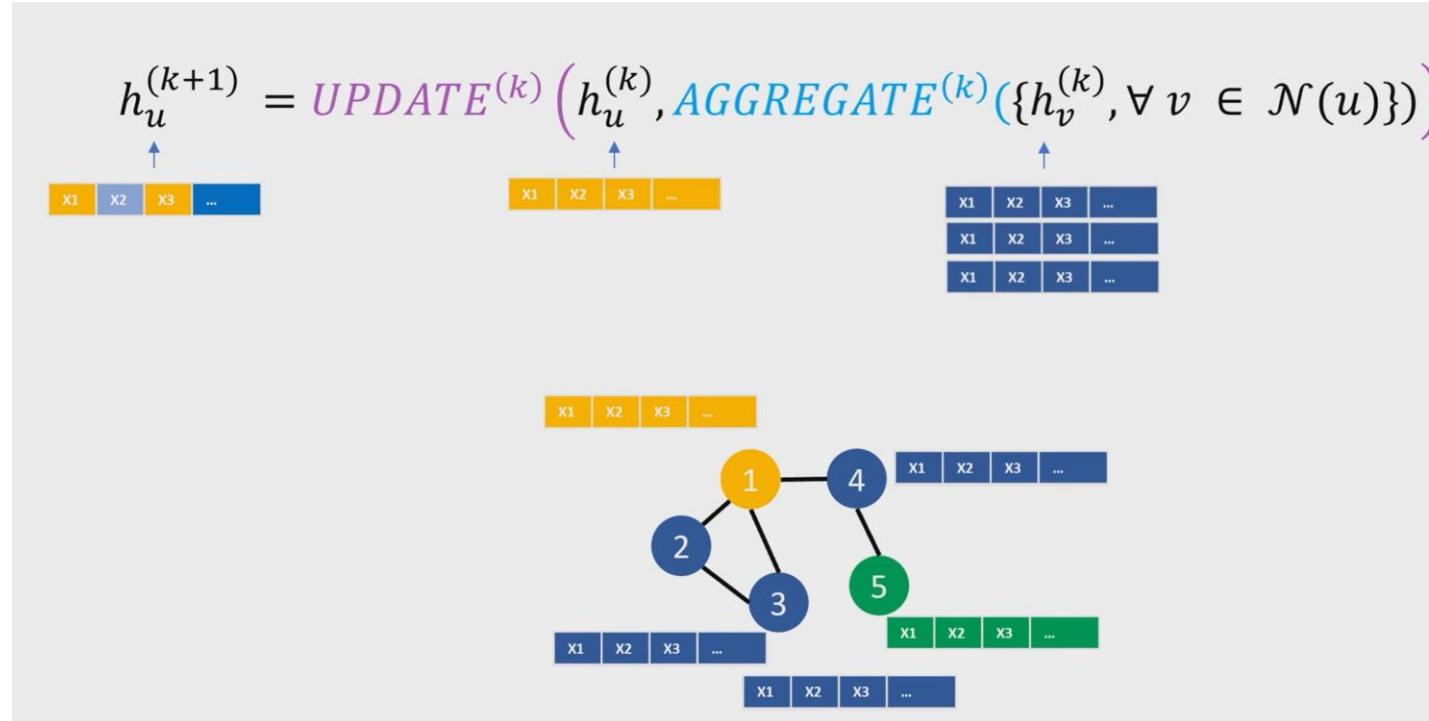
Graph Neural Networks (cont'd)





Message Passing in GNNs

- Message Passing updates and aggregations:



Message Passing in GNNs at a Glance

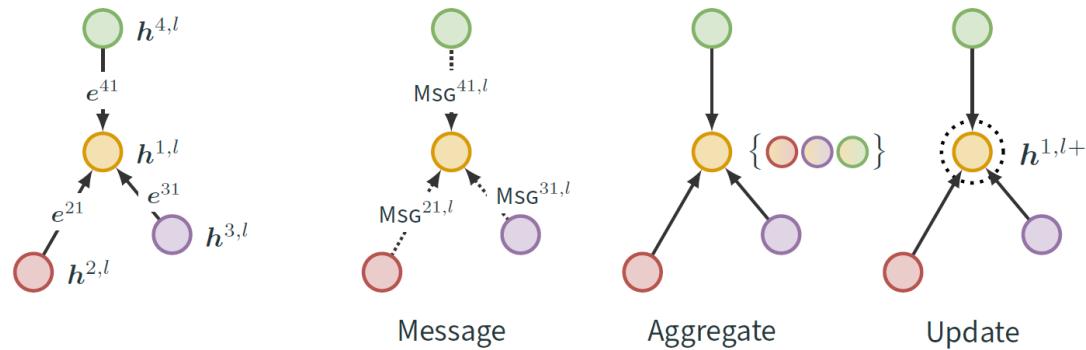
- Number of message-passing layers is a **hyper-parameter**
 - Too many layers → **over-smoothing**



Message Passing in GNNs

To process the spatial dimension, we rely on the **message-passing (MP)** framework

$$\mathbf{h}^{i,l+1} = \text{UP}^l \left(\mathbf{h}^{i,l}, \underset{j \in \mathcal{N}(i)}{\text{AGGR}} \left\{ \text{MSG}^l(\mathbf{h}^{i,l}, \mathbf{h}^{j,l}, e^{ji}) \right\} \right),$$



Where:

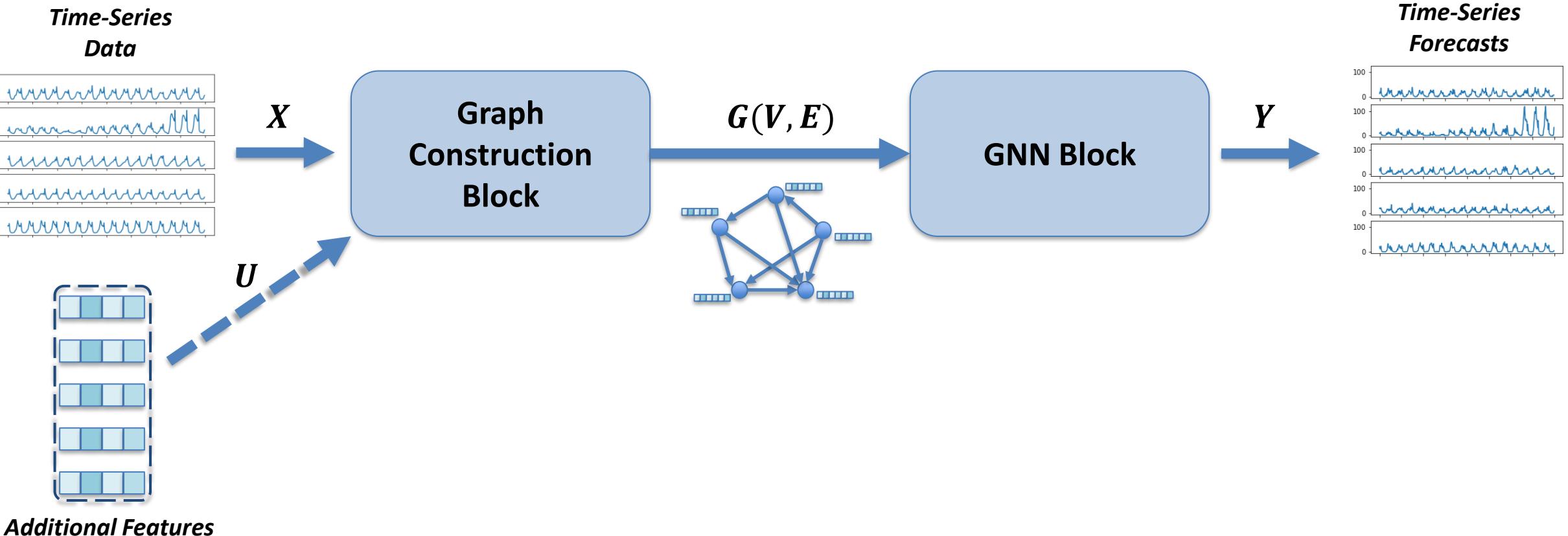
- $\text{MSG}^l(\cdot)$ is the **message function**, e.g., implemented by an MLP.
- $\text{AGGR}\{\cdot\}$ is the permutation invariant **aggregation function**.
- $\text{UP}^l(\cdot)$ is the **update function**, e.g., implemented by an MLP.

Aggregation is performed over $\mathcal{N}(i)$, i.e., the set of neighbors of node i .



GNN-based Time-Series Forecasting

General Framework





DCRNN for Traffic Forecasting

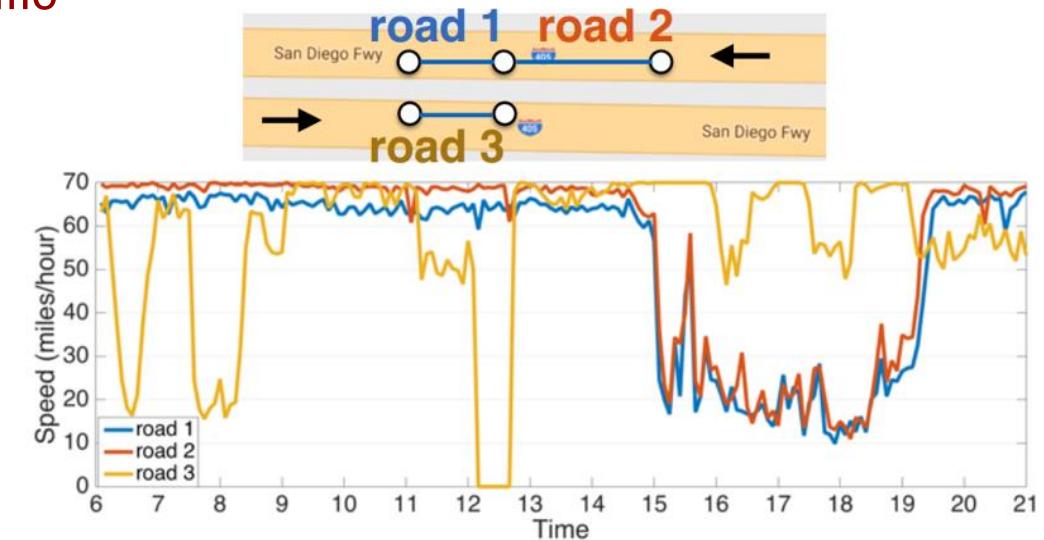


DCRNN for Traffic Forecasting

- **Forecasting Problem:**

$$[\mathbf{X}^{(t-T'+1)}, \dots, \mathbf{X}^{(t)}; \mathcal{G}] \xrightarrow{h(\cdot)} [\mathbf{X}^{(t+1)}, \dots, \mathbf{X}^{(t+T)}]$$

What are some interesting observations from the traffic observations in this figure?





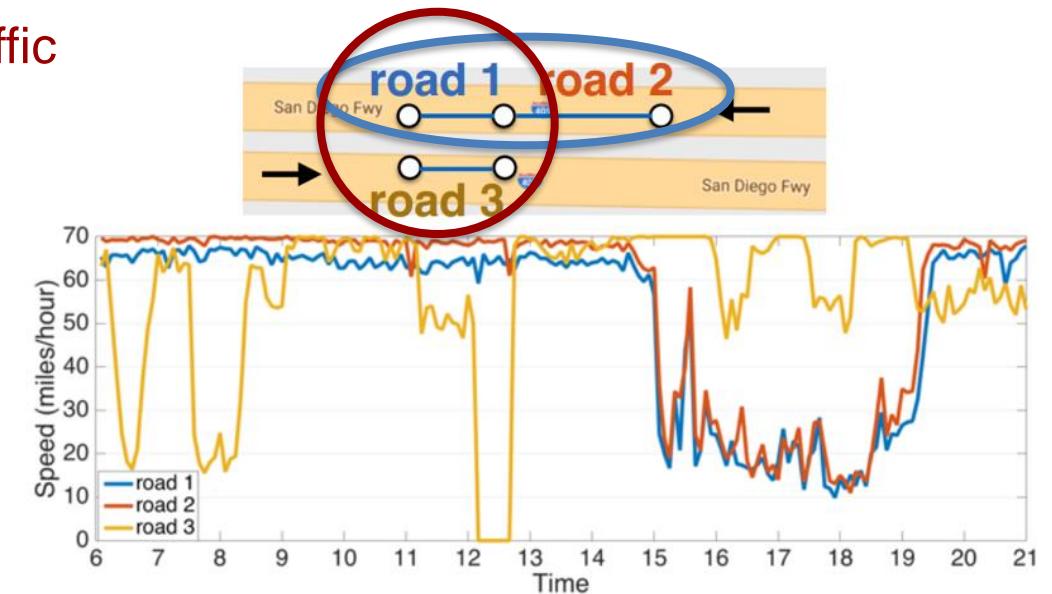
DCRNN for Traffic Forecasting

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What are some interesting observations from the traffic observations in this figure?

1. **Complex spatial dependencies:** Traffic patterns show **non-Euclidean** dependencies



DCRNN for Traffic Forecasting



- **Forecasting Problem:**

$$[\mathbf{X}^{(t-T'+1)}, \dots, \mathbf{X}^{(t)}; \mathcal{G}] \xrightarrow{h(\cdot)} [\mathbf{X}^{(t+1)}, \dots, \mathbf{X}^{(t+T)}]$$

What are some interesting observations from the traffic observations in this figure?

2. **Non-linear temporal dynamics:** Rush hours and traffic incidents causes **non-stationarity**



DCRNN for Traffic Forecasting

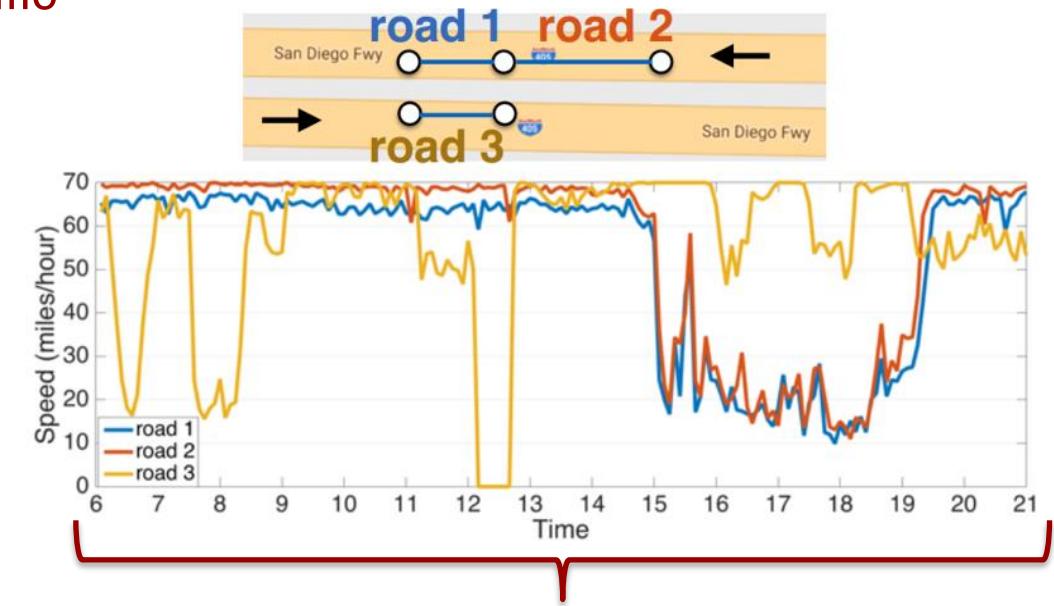


- **Forecasting Problem:**

$$[\mathbf{X}^{(t-T'+1)}, \dots, \mathbf{X}^{(t)}; \mathcal{G}] \xrightarrow{h(\cdot)} [\mathbf{X}^{(t+1)}, \dots, \mathbf{X}^{(t+T)}]$$

What are some interesting observations from the traffic observations in this figure?

3. **Difficulty of long-term forecasting:** Traffic measurements **fluctuate** heavily during a long window



DCRNN for Traffic Forecasting – Overall Framework



Diffusion Convolutional Recurrent Neural Network: Data-Driven Traffic Forecasting

Goal: Vehicle traffic forecasting

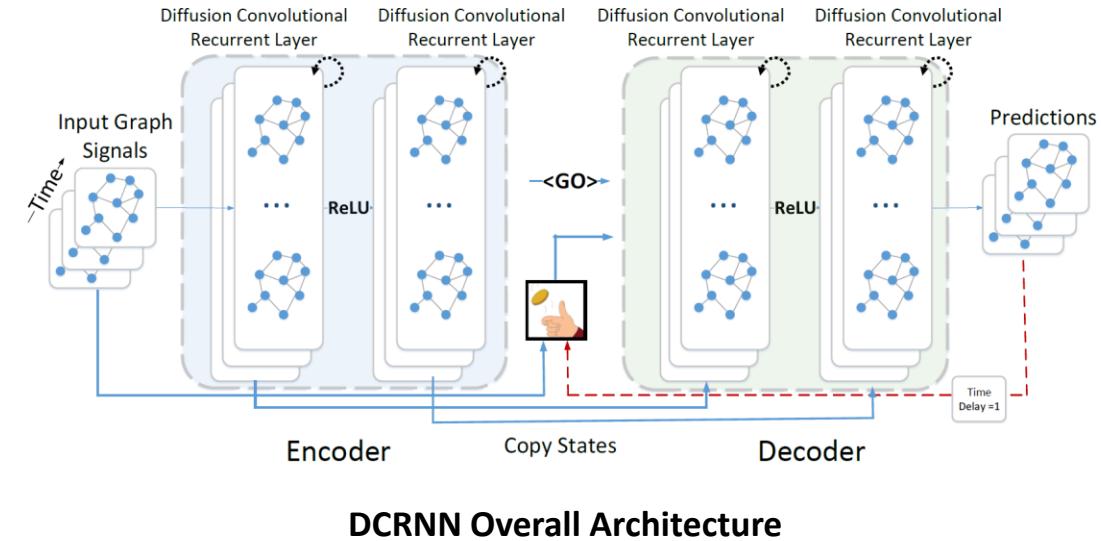
Graph Construction Block: Building a **static graph** of traffic sensors based on their road-network distances

GNN Block: Applying **Graph Diffusion Convolution** with a **seq-to-seq** architecture on the previous graph utilizing the following techniques:

Diffusional Convolution: To capture complex spatial dependencies

Recurrent Neural Networks: To capture non-linear temporal dynamics

Encoder-Decoder Architecture: To capture better long-term dependencies



DCRNN Overall Architecture



DCRNN – Graph Construction

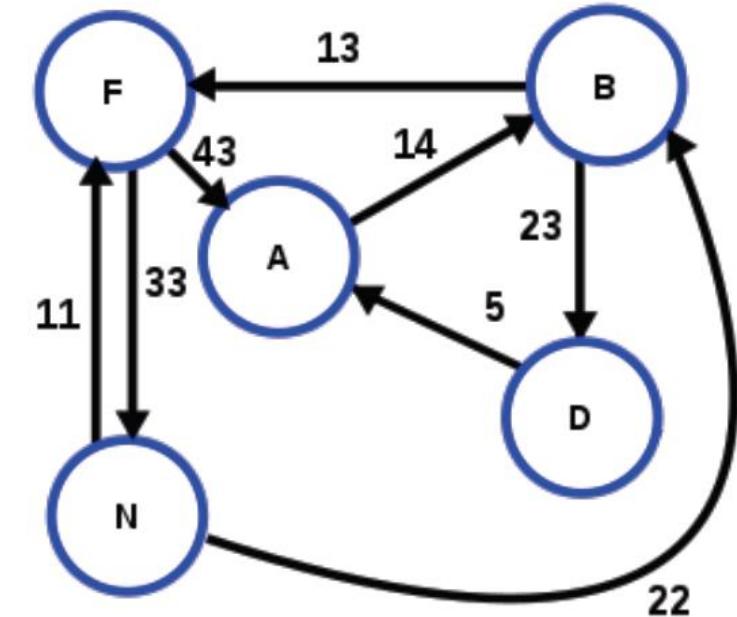
Graph Construction: Based on the **road-network distance** between traffic sensors

- Transportation network as graph
 - V = Vertices (sensors)
 - E = Edges (roads)
 - A = Weighted adjacency matrix
(A function of the road network distance)

$$A_{ij} = \exp\left(-\frac{\text{dist}_{\text{net}}(v_i, v_j)^2}{\sigma^2}\right) \text{ if } \text{dist}_{\text{net}}(v_i, v_j) \leq \kappa$$

$\text{dist}_{\text{net}}(v_i, v_j)$: road network distance from v_i to v_j ,

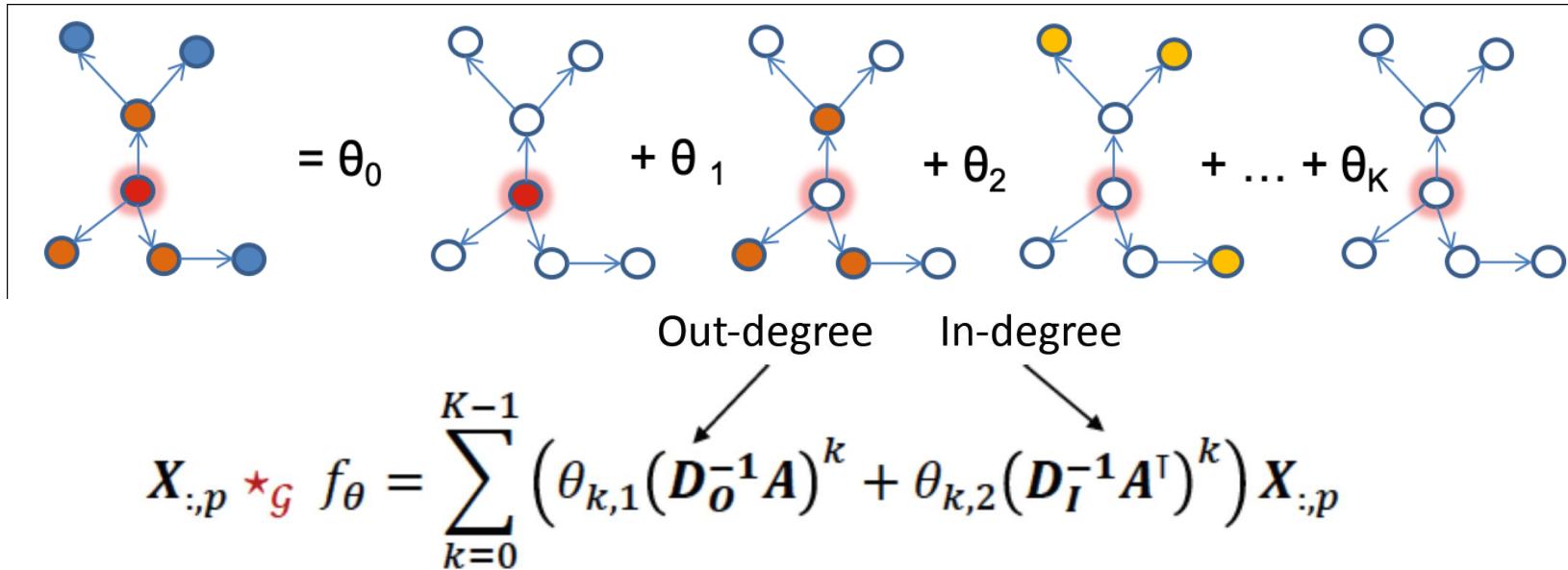
κ : threshold to ensure sparsity, σ^2 variance of all pairwise road network distances





DCRNN – GNN Block

Diffusion Convolution



- $\theta \in \mathbb{R}^{K \times 2}$ are the parameters to train
- A is the adjacency matrix (previous page)
- $X \in \mathbb{R}^{N \times P}$ is the input with N as the # of nodes, P as the feature dimension of each node
- D_O : Out-degree matrix for outgoing flow / D_I : In-degree matrix for incoming flow



DCRNN – GNN Block

Diffusion Convolution

- Take $K = 3$ for example
- Note – Change of notation: \mathbf{W} now represents the adjacency matrix (previously denoted as A in earlier slides).

$$\sum_{k=0}^{K-1} \theta_{k,1} (D_O^{-1} \mathbf{W})^k \mathbf{X}_{:,p} = \boxed{\theta_{0,1} \mathbf{X}_{:,p}} + \theta_{1,1} (D_O^{-1} \mathbf{W})^1 \mathbf{X}_{:,p} + \theta_{1,2} (D_O^{-1} \mathbf{W})^2 \mathbf{X}_{:,p}$$



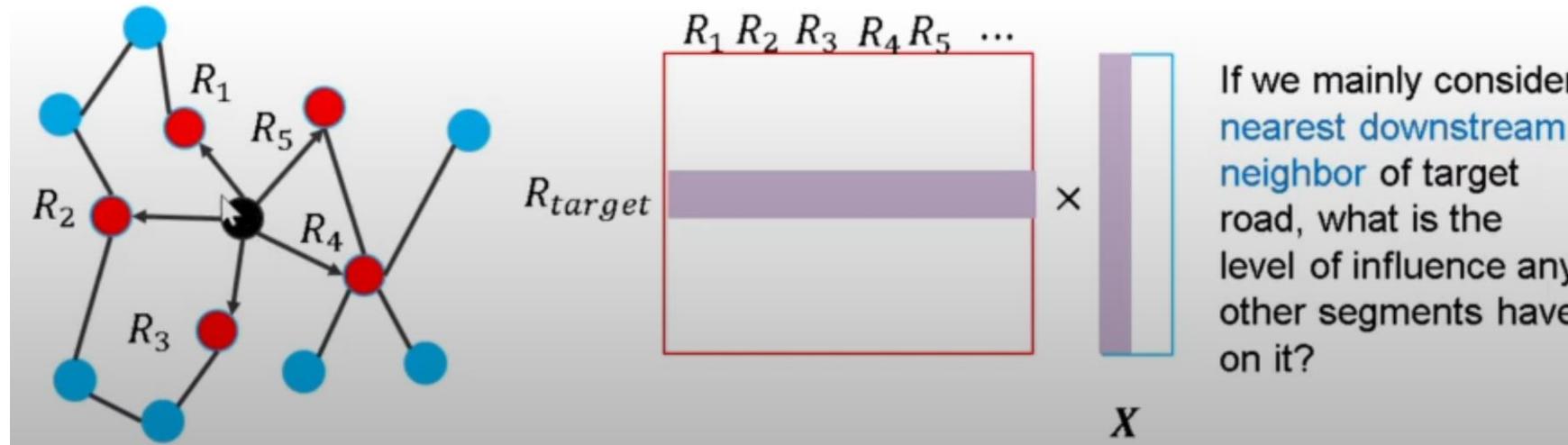


DCRNN – GNN Block

Diffusion Convolution

- Take $K = 3$ for example
- Note – Change of notation: W now represents the adjacency matrix (previously denoted as A in earlier slides).

$$\sum_{k=0}^{K-1} \theta_{k,1} (D_O^{-1} W)^k X_{:,p} = \theta_{0,1} X_{:,p} + \boxed{\theta_{1,1} (D_O^{-1} W)^1 X_{:,p}} + \theta_{1,2} (D_O^{-1} W)^2 X_{:,p}$$



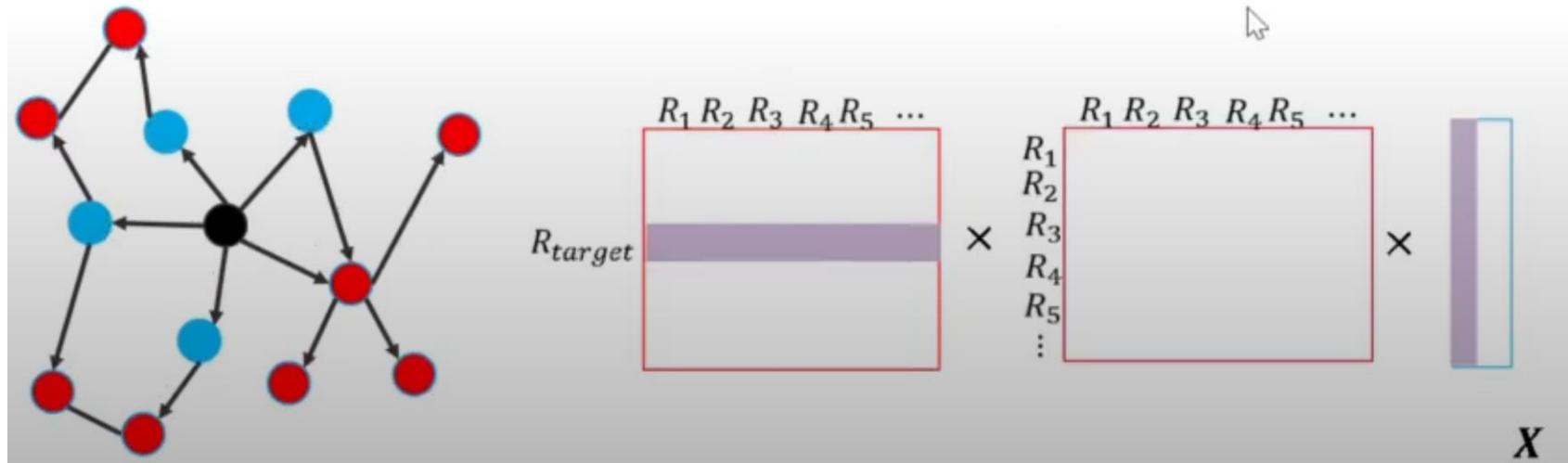


DCRNN – GNN Block

Diffusion Convolution

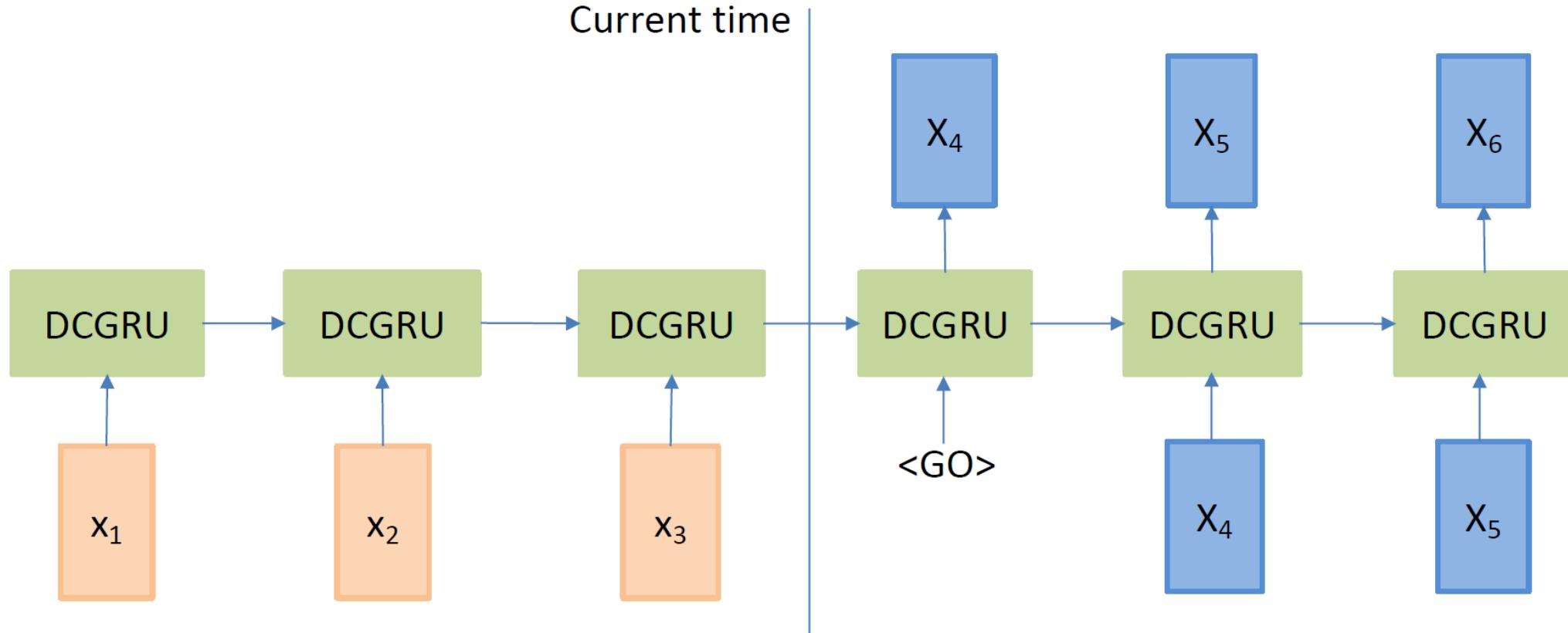
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$$\sum_{k=0}^{K-1} \theta_{k,1} (D_O^{-1} \mathbf{W})^k \mathbf{X}_{:,p} = \theta_{0,1} \mathbf{X}_{:,p} + \theta_{1,1} (D_O^{-1} \mathbf{W})^1 \mathbf{X}_{:,p} + \boxed{\theta_{1,2} (D_O^{-1} \mathbf{W})^2 \mathbf{X}_{:,p}}$$





Encoder-Decoder Framework of DCRNN





Encoder-Decoder Framework of DCRNN

- In DCRNN, the standard **matrix multiplication** in **GRU** is replaced with a **diffusion convolution** operation to capture spatial dependencies in the graph.

GRU Cell

$$u_t = \sigma(w_u[h_{t-1}, x_t])$$

$$r_t = \sigma(w_r[h_{t-1}, x_t])$$

$$c_t = \tanh(w_c[r_t * h_{t-1}, x_t])$$

$$h_t = (1 - u_t) * h_{t-1} + u_t * c_t$$

DCRNN Cell

$$u_t = \sigma(w_{u*G}[h_{t-1}, x_t])$$

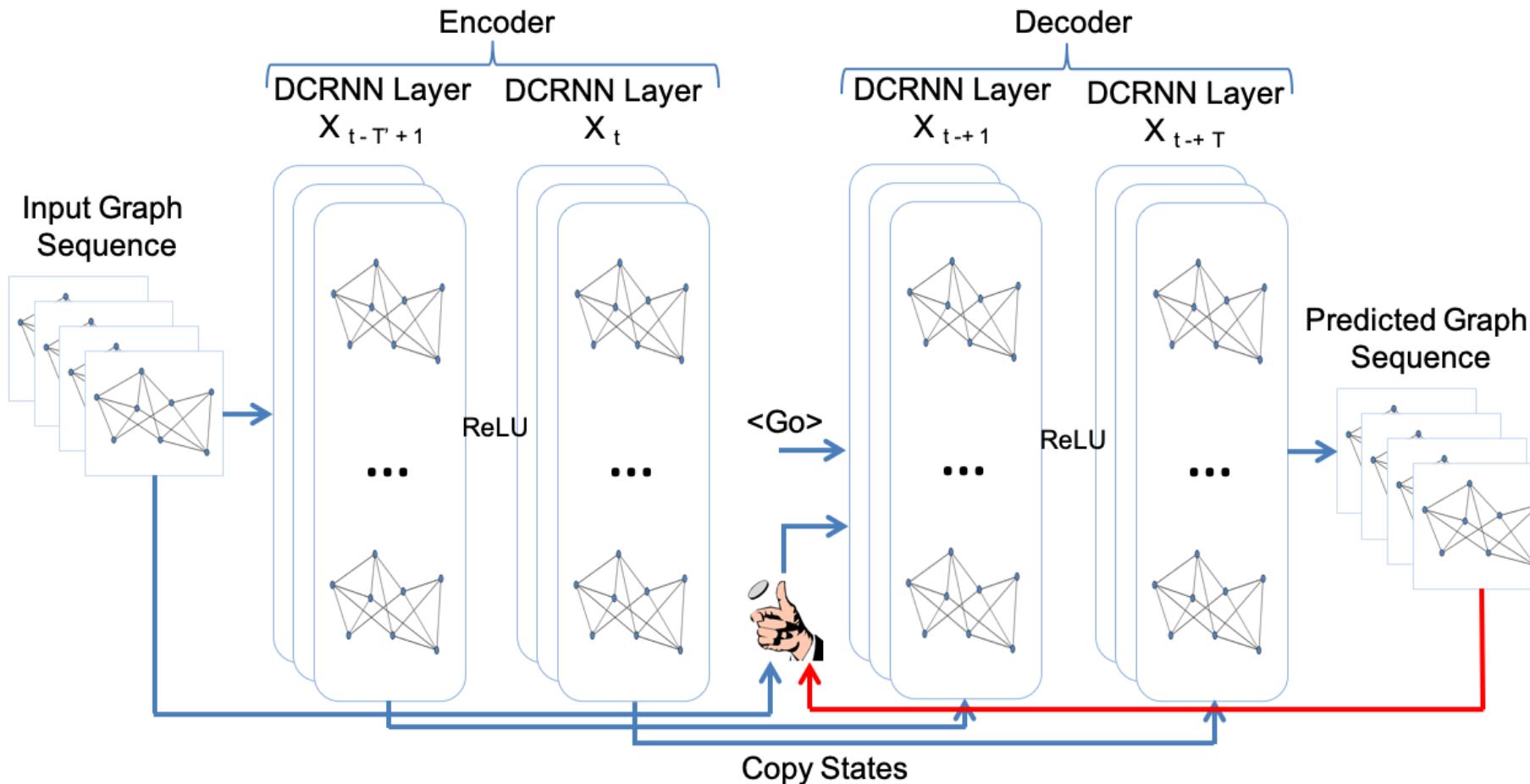
$$r_t = \sigma(w_{r*G}[h_{t-1}, x_t])$$

$$c_t = \tanh(w_{c*G}[r_t * h_{t-1}, x_t])$$

$$h_t = (1 - u_t) * h_{t-1} + u_t * c_t$$



DCRNN End-to-End Framework





BysGNN for Traffic Forecasting

Business Graph Neural Network – Motivation



- **Limitations of Static Models (e.g., DCRNN):** **Fixed graphs** miss the **changing nature** of traffic and **context**-based correlations (e.g., road type).
- **Need for Dynamic Adaptation:** Effective forecasting requires capturing both **static** and **dynamic** relationships between sensors.
- **BysGNN's Goal:** Create a model that **dynamically** learns these relationships to improve traffic prediction accuracy.

BysGNN – Definitions



Definition 1: Multi-Context Correlations

Latent relationships among traffic sensors that are influenced by various contextual factors, including:

- **Spatial correlations:** closeness of **geographical** sensor locations.
- **Temporal dependencies:** the changes in visit patterns of individual sensor observations over time (**intra-series**) and the dependencies between traffic patterns of different sensors (**inter-series**).
- **Semantic similarities:** Similarity of sensor **attributes**, such as their road types (e.g., highway/arterial).
- **Taxonomic correlations:** Similarities in traffic patterns of different **groups of sensors**, e.g., similarities between **high-level** traffic observed in two different neighborhoods.

BysGNN – Definitions



Definition 2: Busyness Graph

- A graph $G = (V, A)$ where V is a set of $|V| = N$ nodes, and each node corresponds to a specific traffic sensor or a group of traffic sensors (e.g., all sensors in West Hollywood).
- We denote $A \in \mathbb{R}^{N \times N}$ as the adjacency matrix in which a_{ij} indicates the amount of influence that node v_i has on the forecasts of v_j .
- Adjacency matrix A is dynamically updated based on the Multi-Context Correlations and captures the most recent knowledge about interaction between traffic sensors.

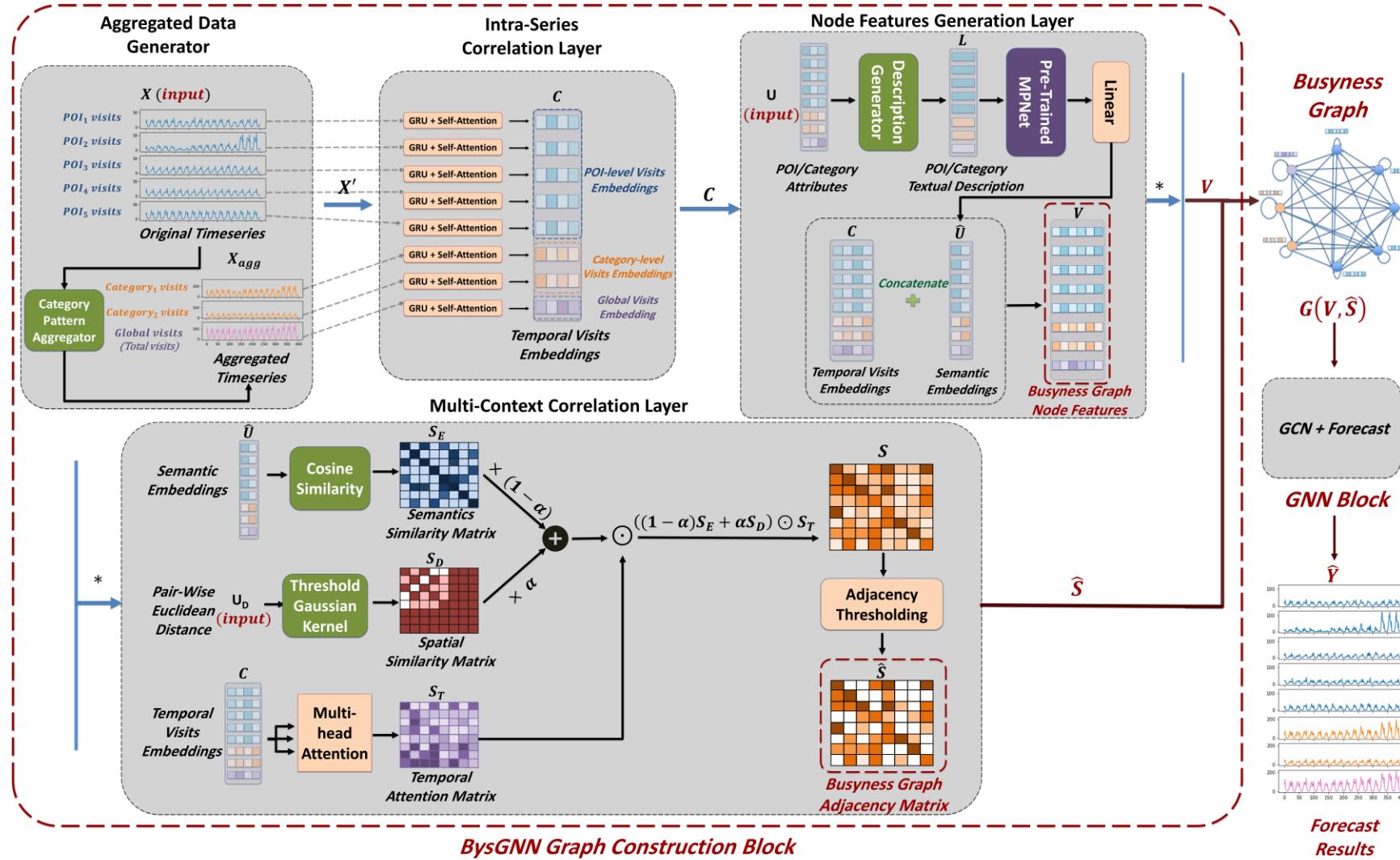
BysGNN – Traffic Forecasting Problem



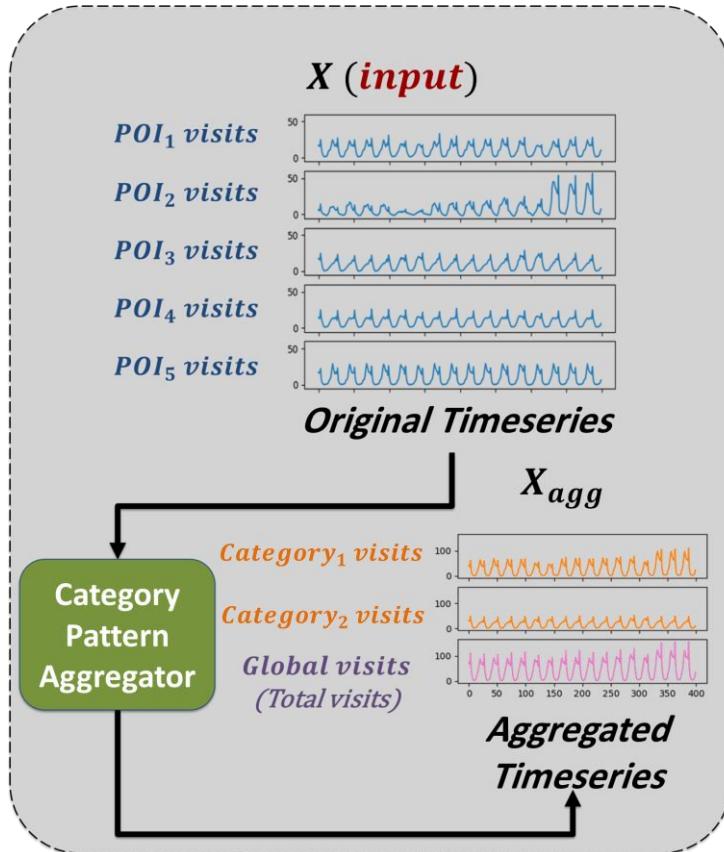
Traffic Forecasting Problem:

Given $\mathbf{X} = (x_1, \dots, x_n) \in \mathbb{R}^{N \times T}$ as the sequence of traffic measurements for the past T hours to N sensors, and $\mathbf{U} = (u_1, \dots, u_N) \in \mathbb{R}^{N \times J}$ as the set of J attributes (e.g., road type, number of lanes, etc.) of each traffic sensor, generate Busyness Graph G to find $\mathbf{Y} = (y_1, \dots, y_N) \in \mathbb{R}^{N \times H}$, the future traffic measurements for the next H time steps for each sensor.

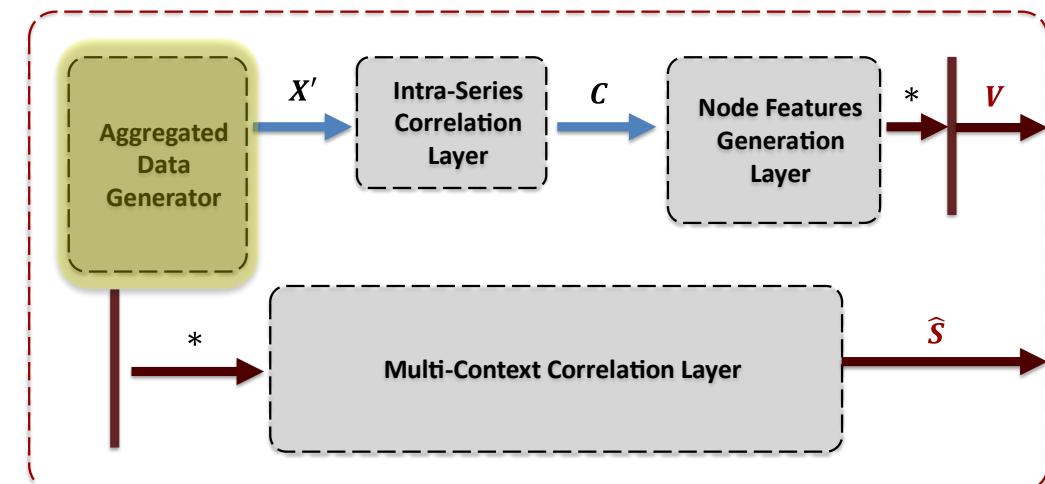
Busyness Graph Neural Network (BysGNN) Framework



BysGNN Framework – Aggregated Data Generator

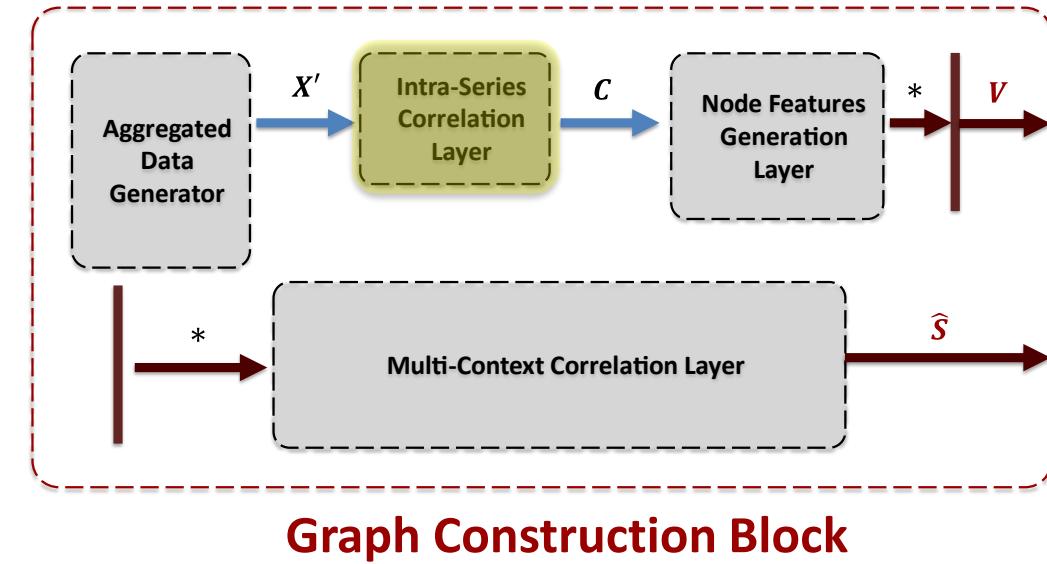
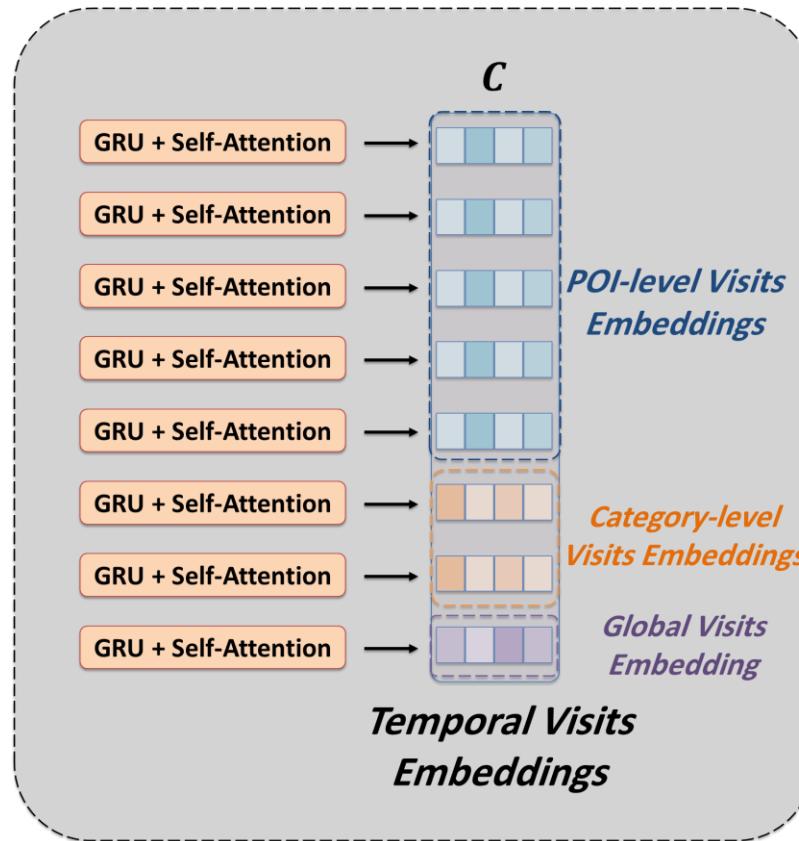


To adapt this framework for traffic forecasting, aggregated series are generated by **aggregating sensors from each geographical neighborhood**

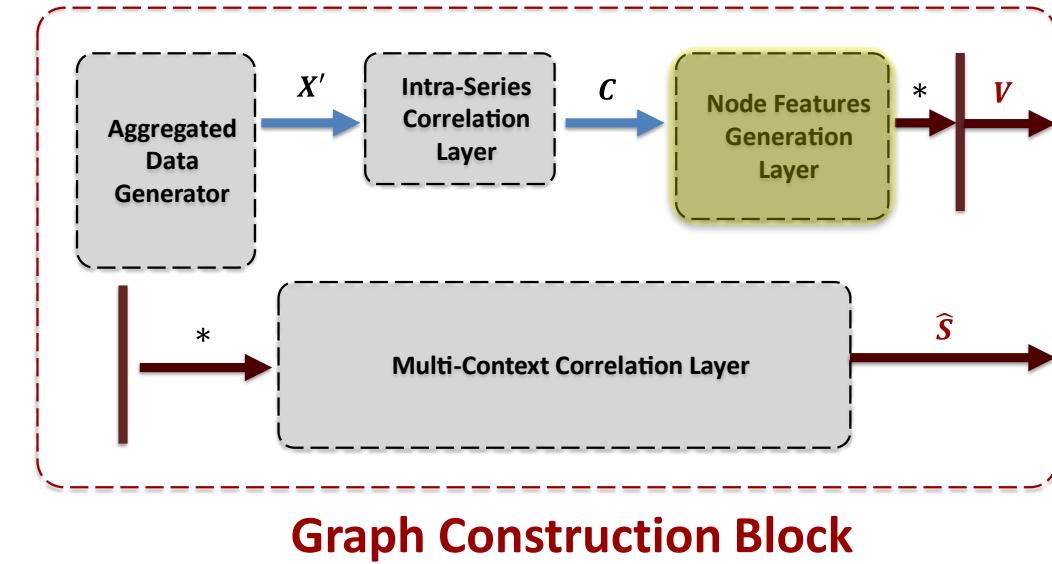
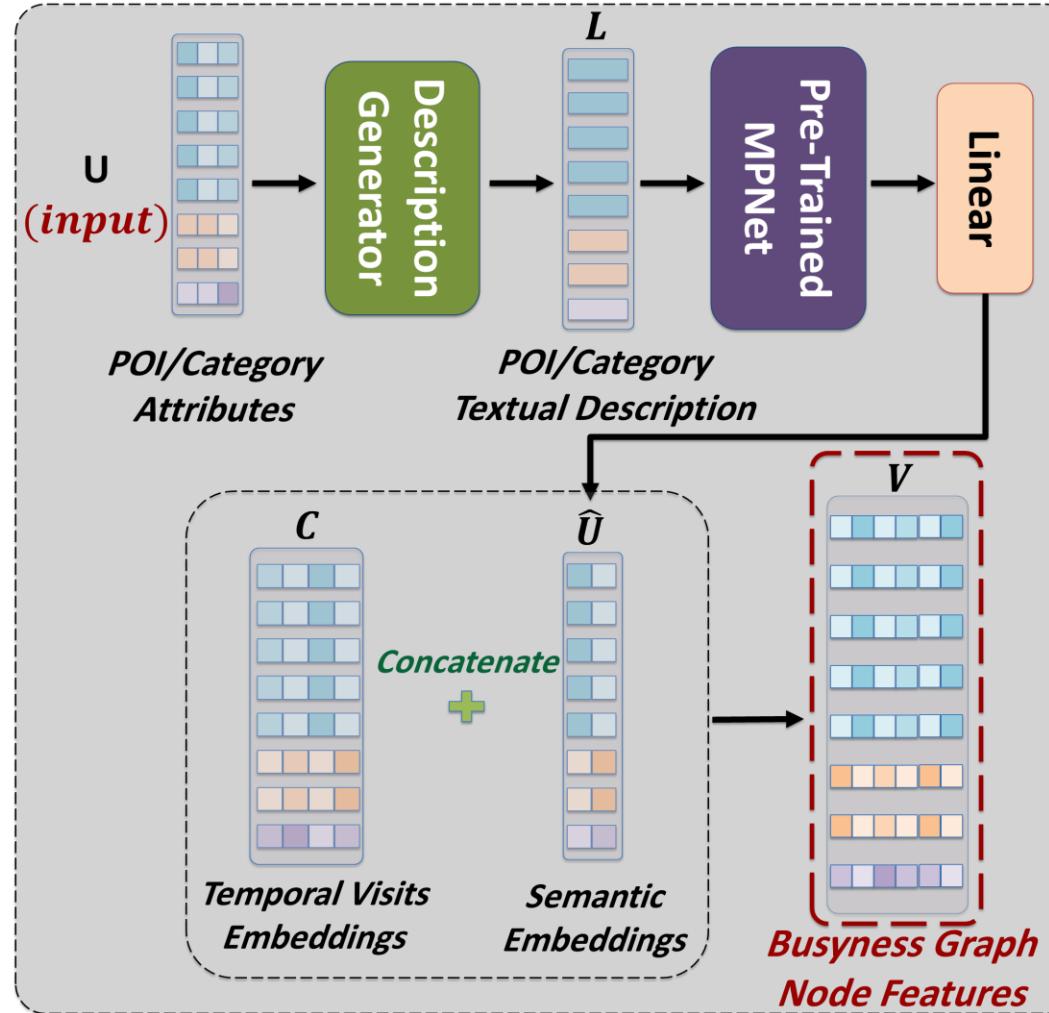


Graph Construction Block

BysGNN Framework – Intra-Series Correlation Layer



BysGNN Framework – Node Features Generation Layer

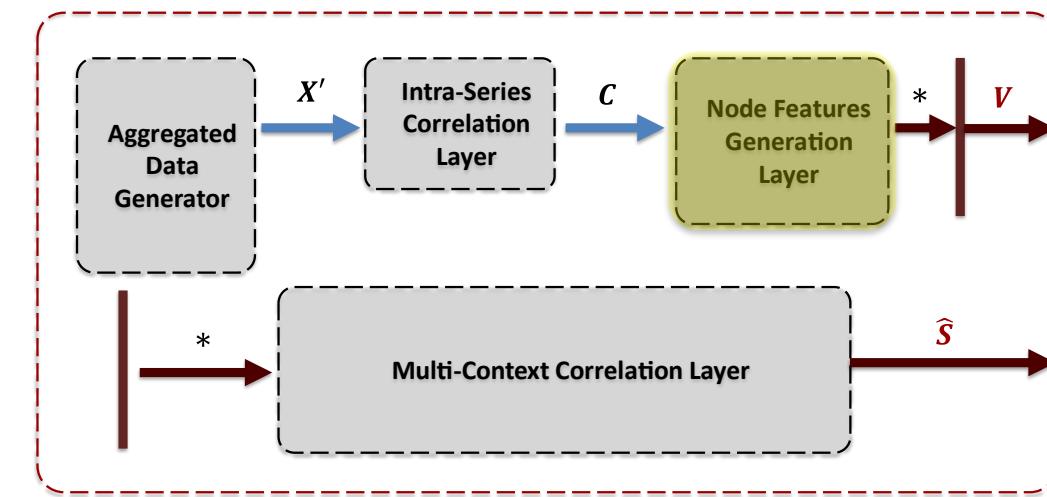


BysGNN Framework – Node Features Generation Layer



Sample Generated Textual Description for a traffic sensor:

This arterial road on **Main St., Los Angeles, CA**, has **3 lanes** with a **max speed limit of 45 mph**. Peak traffic occurs **weekdays from 7:00 - 9:00 AM and 4:00 - 6:00 PM**. It primarily serves **commuter traffic**, classified under **Urban Roads** and **High-Traffic Zones**.

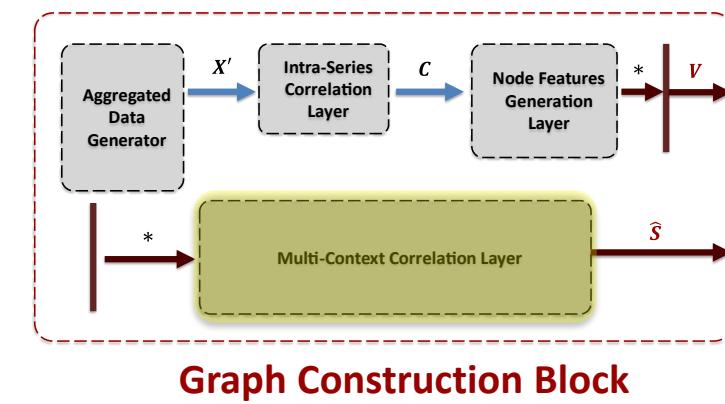
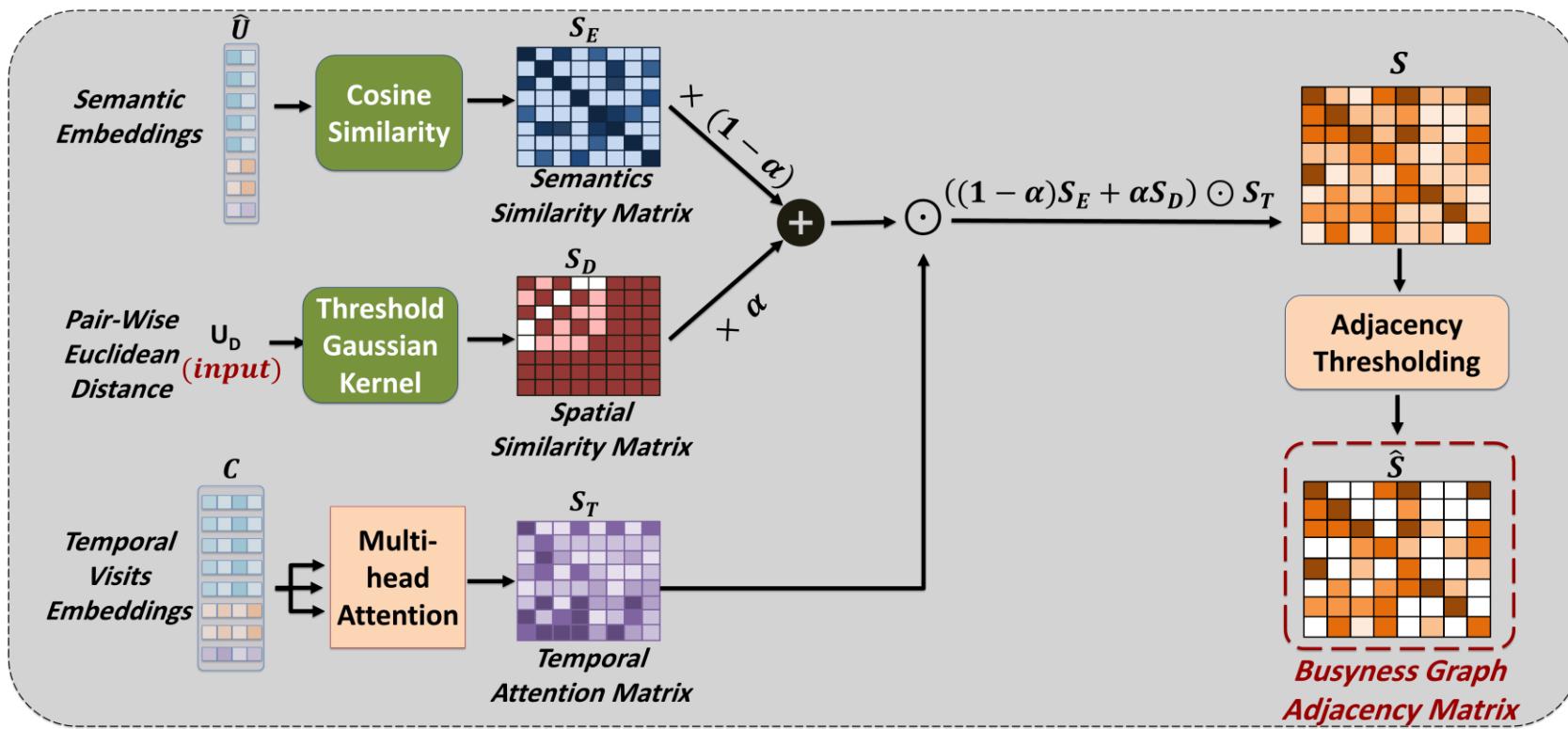


Graph Construction Block

Sample Generated Textual Description for a Category:

This neighborhood is a **commercial district**, experiencing high traffic volumes due to **commuter and shopping traffic**. Primary access routes include **Broadway and Main St.**

BysGNN Framework – Multi-Context Correlation Layer



BysGNN Framework – Multi-Context Correlation Layer (cont'd)



Gating Mechanism:

Helps to preserve strong long-term relationships and penalize noisy relationships between distant or semantically dissimilar nodes

Adjacency Thresholding:

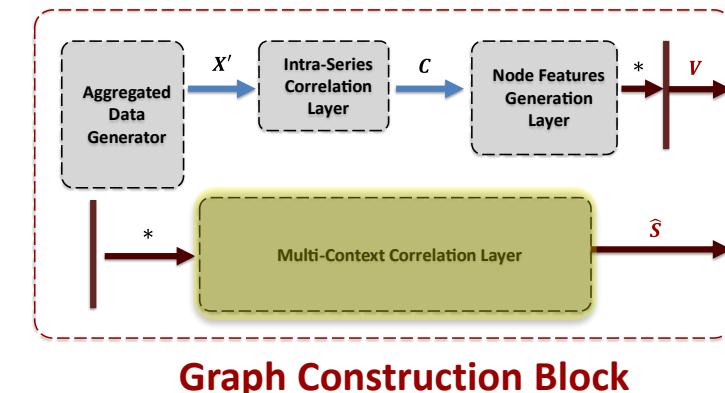
Filters out the previous noisy relationships.

BysGNN uses a case amplification function to differentiate between small and large values in adjacency matrix. This reduces the impact of small values more significantly than the larger values. This is done as follows:

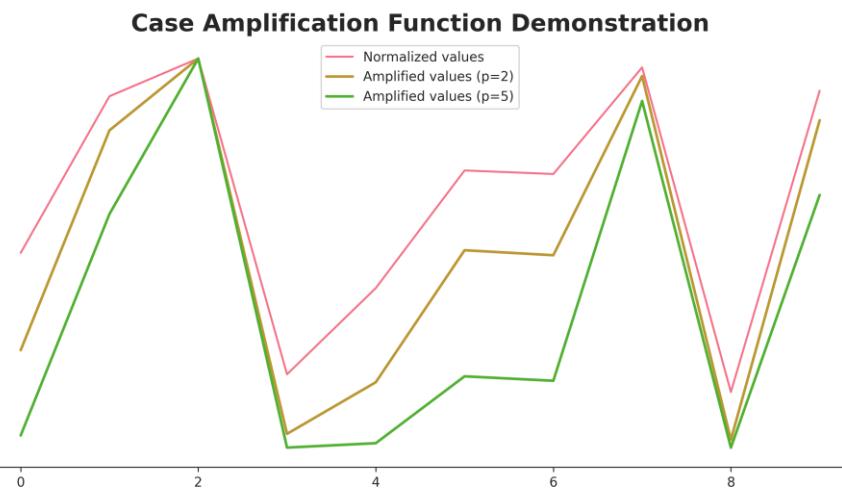
S : Original Adjacency Matrix

\hat{S} : Thresholded Adjacency Matrix

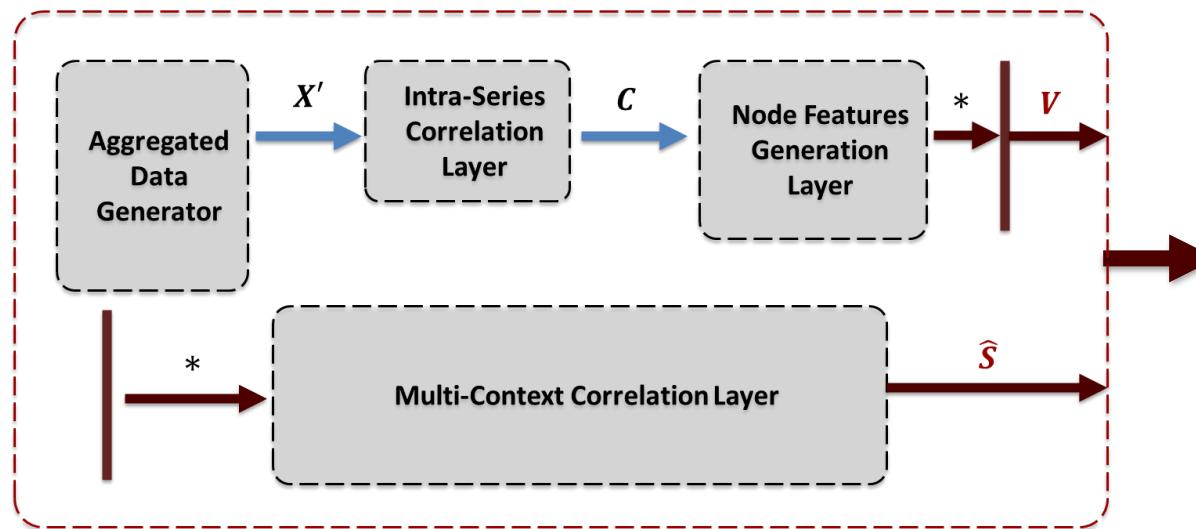
$$\hat{S}_{ij} = \begin{cases} S_{ij}, & \text{if } \left(\frac{S_{ij}}{\max(S_i)}\right)^p > \eta \\ 0, & \text{otherwise} \end{cases}$$



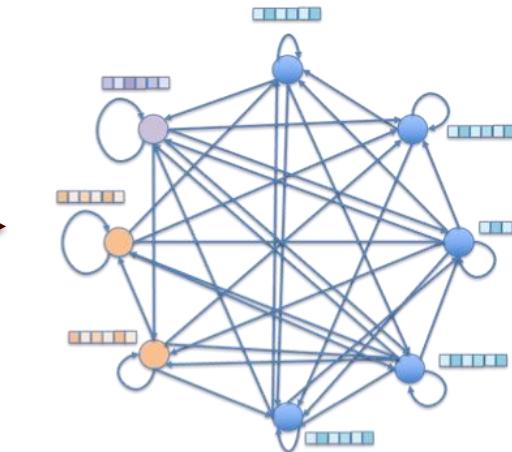
Graph Construction Block



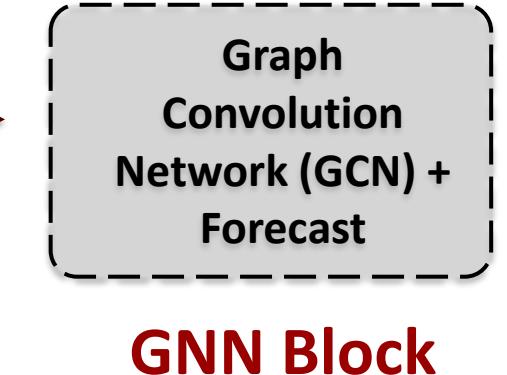
BysGNN – Busyness Graph and GNN Block



**Graph Construction
Block**



Busyness Graph



GNN Block

Traffic Forecasting Evaluation



Task: Forecast the # of visits to each POI for the **next 6 hours** from the **past 24 hours** of visitation data

Evaluation Metrics

MAE: Average of the difference between the ground truth and the predicted values

$$MAE = \frac{1}{N} \sum_{j=1}^N |y_j - \hat{y}_j|$$

MAPE: the percentage equivalent of MAE

$$MAPE = \frac{100\%}{N} \sum_{j=1}^N \left| \frac{y_j - \hat{y}_j}{y_j} \right|$$

RMSE: Square root of the average of the squared difference between the target value and the value predicted

$$RMSE = \sqrt{\frac{1}{N} \sum_{j=1}^N (y_j - \hat{y}_j)^2}$$



Experiments Results – Large Data Regime

Evaluation

- BySGNN significantly outperforms DCRNN
- ...demonstrating that **dynamically capturing relationships** yields **better** results than relying on a **fixed, predefined** structure.

Forecasting Results for High # of POIs Data Regime

Dataset Evaluation Metric	Houston			Los Angeles			New York		
	MAE	MAPE	RMSE	MAE	MAPE	RMSE	MAE	MAPE	RMSE
Naïve Seasonal	4.746	0.664	18.166	2.934	0.752	10.005	3.681	0.699	9.216
Historical Average	8.860	0.783	26.911	4.388	0.786	11.729	6.555	0.770	22.018
ConvGRU	6.415	2.539	20.179	3.781	3.139	10.905	4.605	1.851	17.028
ConvLSTM	8.076	4.270	23.127	4.362	4.397	11.879	5.448	2.697	18.959
DCRNN	5.683	1.990	18.941	3.389	2.693	9.879	4.139	1.605	15.504
A3T-GCN	8.380	3.377	23.9	4.604	4.129	12.601	5.824	2.579	20.171
StemGNN	4.390	0.735	14.604	2.485	0.671	6.951	3.261	0.652	8.074
BysGNN	4.095	0.658	12.904	2.377	0.676	6.091	3.113	0.598	7.351
RelError	-6.71%	-0.90%	-11.64%	-4.34%	+0.74%	-12.37%	-4.53%	-8.28%	-8.95%

Dataset Evaluation Metric	Chicago			San Antonio		
	MAE	MAPE	RMSE	MAE	MAPE	RMSE
Naïve Seasonal	3.237	0.754	9.216	3.85	0.689	10.573
Historical Average	4.624	0.791	14.011	6.494	0.78	15.776
ConvGRU	4.18	2.675	10.753	4.622	2.838	10.218
ConvLSTM	5.019	3.853	11.972	5.745	5.202	11.608
DCRNN	3.756	2.327	9.857	4.167	2.269	9.513
A3TGNCN	5.343	3.654	12.821	6.086	4.517	12.731
StemGNN	2.776	0.724	9.857	3.371	0.686	8.923
BysGNN	2.750	0.718	8.218	3.278	0.629	8.418
RelError	-0.93%	-0.82%	-10.82%	-2.75%	-8.30%	-5.65%

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