

# Graph Neural Network

Temporal and Spatial Air Pollution Measurement Station

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Phiphat Chomchit

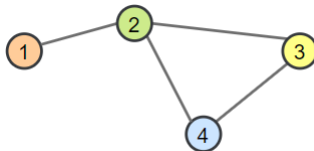
CMU

# What is Graph Neural Network?

## Graph definition

A graph  $\mathcal{G}$  is defined as a tuple of a set of nodes/vertices  $V$ , and a set of edges /links  $E$ :  $\mathcal{G} = (V, E)$ . Each edge is a pair of two vertices, and represents a connection between them.

For instance, let's look at the following graph:



The vertices are  $V = \{1, 2, 3, 4\}$ ,  
and edges  $E = \{(1, 2), (2, 3), (2, 4), (3, 4)\}$ .

# What is Graph Neural Network?

## Definition of Adjacency Matrix

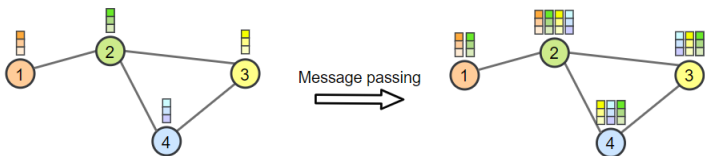
The **adjacency matrix**  $A$  is a square matrix whose elements indicate whether pairs of vertices are adjacent, i.e. connected, or not. In the simplest case,  $A_{ij}$  is 1 if there is a connection from node  $i$  to  $j$ , and otherwise 0.

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

keep in mind that  $A$  is a symmetric matrix ( $A_{ij} = A_{ji}$ )

# Graph Convolutions

1. GCNs are similar to convolutions in images in the sense that the "filter" parameters are typically shared over all locations in the graph.
2. At the same time, GCNs rely on message passing methods, which means that vertices exchange information with the neighbors, and send "messages" to each other.



# Graph Convolutions

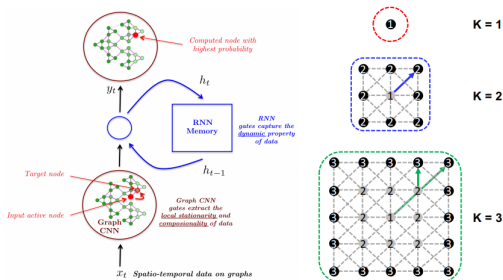
Given the previous features of nodes  $H^{(l)}$ , the GCN layer is defined as follows:

$$H^{(l+1)} = \sigma \left( \hat{D}^{-1/2} \hat{A} \hat{D}^{-1/2} H^{(l)} W^{(l)} \right)$$

1.  $W^{(l)}$  is the weight parameters with which we transform the input features into messages ( $H^{(l)} W^{(l)}$ ).
2. To the adjacency matrix  $A$  we add the identity matrix so that each node sends its own message also to itself:  $\hat{A} = A + I$ .
3.  $\hat{D}$  which is a diagonal matrix with  $D_{ii}$  denoting the number of neighbors node  $i$  has.
4.  $\sigma$  represents an arbitrary activation function.

# Structured Sequence Modeling with Graph Convolutional Recurrent Networks

GCRN model modeling and predicting time-varying graph-based data. The core idea is to merge CNN for graph-structured data and RNN to identify simultaneously meaningful spatial structures and dynamic patterns. A generic illustration of the proposed GCRN architecture is given by.



# Structured Sequence Modeling with Graph Convolutional Recurrent Networks

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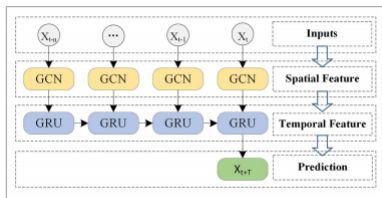


Fig. 3. Overview. We take the historical traffic information as input and obtain the finally prediction result through the Graph Convolution Network and the Gated Recurrent Units model.

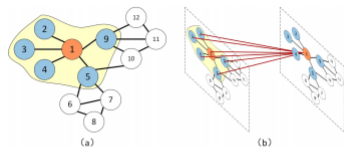
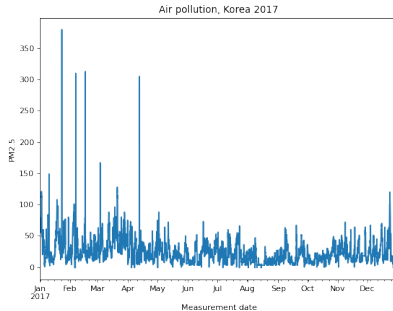


Fig. 4. Assuming that node 1 is a central road. (a) The blue nodes indicate the roads connected to the central road. (b) We obtain the spatial feature by obtaining the topological relationship between the road 1 and the surrounding roads.

# PM2.5 datasets

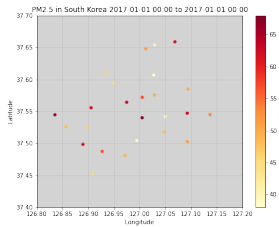
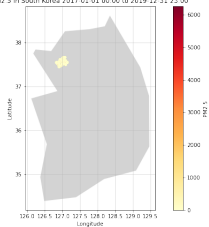
	Measurement date	Station code	Address	Latitude	Longitude	SO2	NO2	O3	CO	PM10	PM2.5
0	2017-01-01 00:00	101	19, Jong-ro 35ga-gil, Jongno-gu, Seoul, Republ...	37.572016	127.005007	0.004	0.059	0.002	1.2	73.0	57.0
1	2017-01-01 01:00	101	19, Jong-ro 35ga-gil, Jongno-gu, Seoul, Republ...	37.572016	127.005007	0.004	0.058	0.002	1.2	71.0	59.0
2	2017-01-01 02:00	101	19, Jong-ro 35ga-gil, Jongno-gu, Seoul, Republ...	37.572016	127.005007	0.004	0.056	0.002	1.2	70.0	59.0
3	2017-01-01 03:00	101	19, Jong-ro 35ga-gil, Jongno-gu, Seoul, Republ...	37.572016	127.005007	0.004	0.056	0.002	1.2	70.0	58.0
4	2017-01-01 04:00	101	19, Jong-ro 35ga-gil, Jongno-gu, Seoul, Republ...	37.572016	127.005007	0.003	0.051	0.002	1.2	69.0	61.0



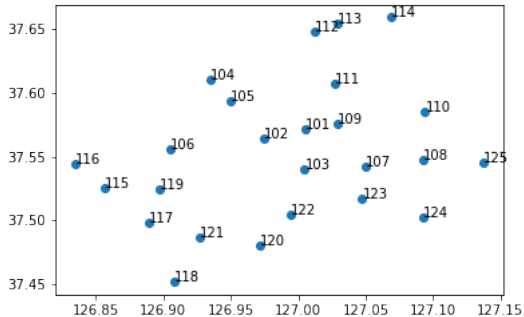


# Stations

PM2.5 in South Korea 2017-01-01 00:00 to 2019-12-31 23:00



# Stations



## Any Question?



**Thnk you!**