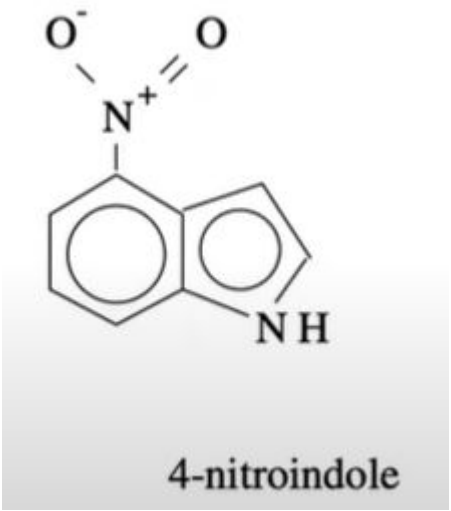
Graph Neural Network

source:http://speech.ee.ntu.edu.tw/~tlkagk/courses/ML2020/GNN.pdf

Why GNN

Chemical problem



→ classifier → The molecular model is valid or not

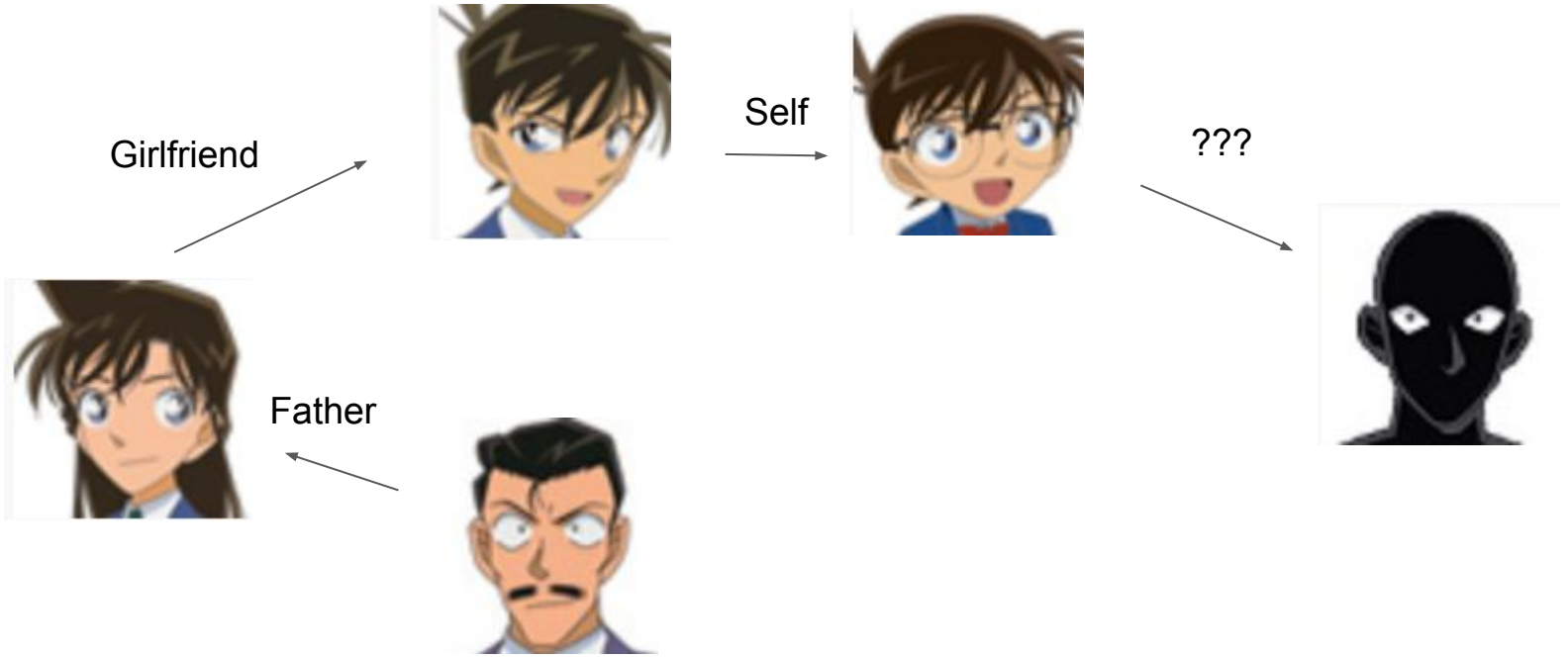
Why GNN

Social network

Node			Feature
	Shinichi Kudo	Jimmy Kudo	Main character of the series, and Ran's love interest and later boyfriend. He was shrunk into a child after being forced to take a drug called APTX 4869, which was created by the Black Organization.
	Conan Edogawa	Conan Edogawa	"Child" version of Shinichi Kudo. He's after the Black Organization to regain his original body. The show follows his journey and the different cases he encounters along the way.
	Ran Mouri	Rachel Moore	Shinichi's childhood friend, and later his girlfriend. She doesn't know Conan's real identity. She's the one taking care of him along with her detective father, Kogoro. She is also skilled in karate.
	Kogoro Mouri	Richard Moore	Private eye and Ran's father. Separated from Eri Kisaki, Ran's mother.

Why GNN

Social network



Why GNN

Social network

F:a person is murder or not

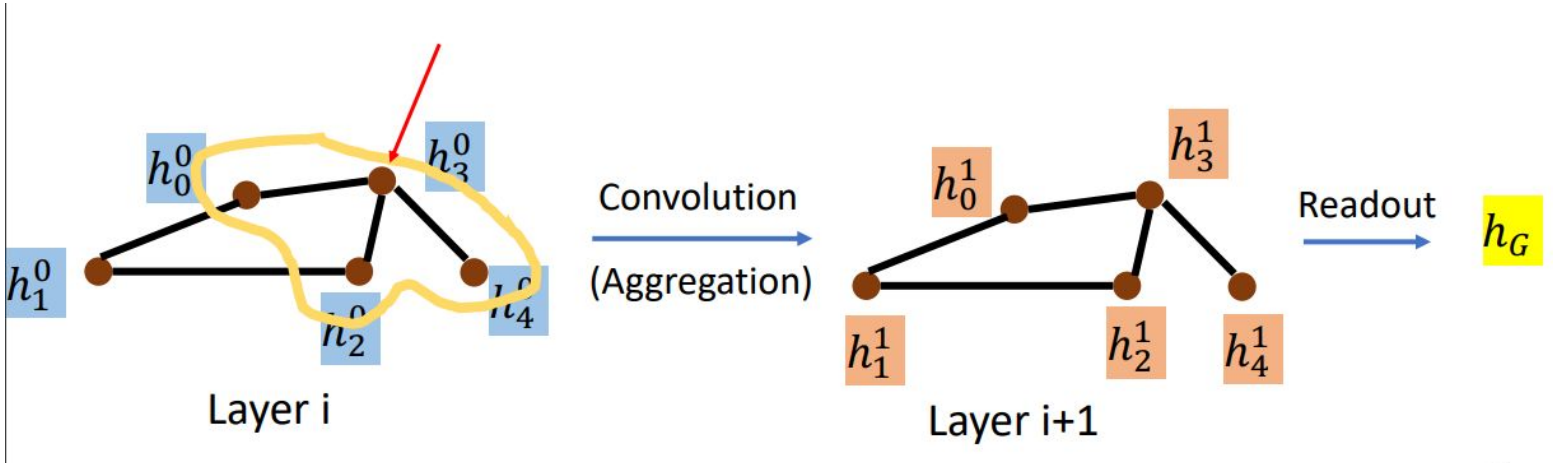
f()-> No

f()-> Yes

Terminology

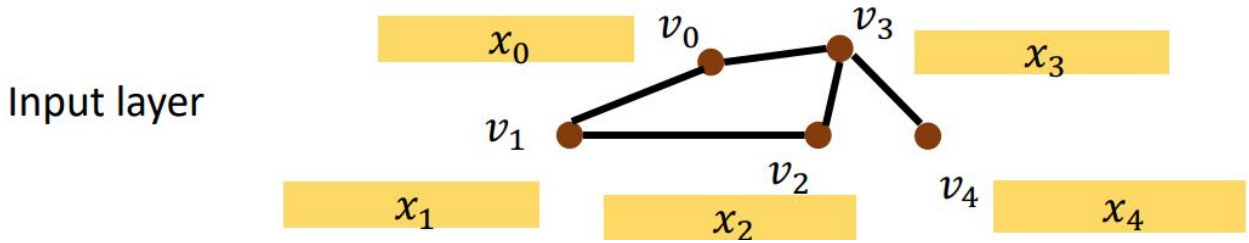
Aggregate: Update the hidden state in next layer by neighborhoods.

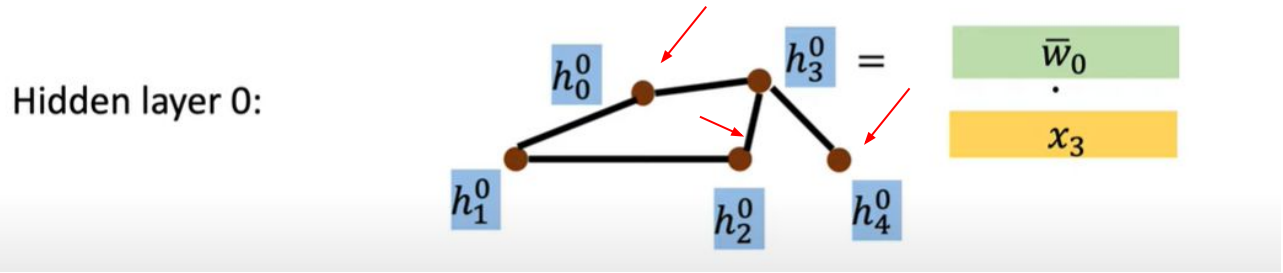
Readout: Combine features of each node to represent the whole graph.

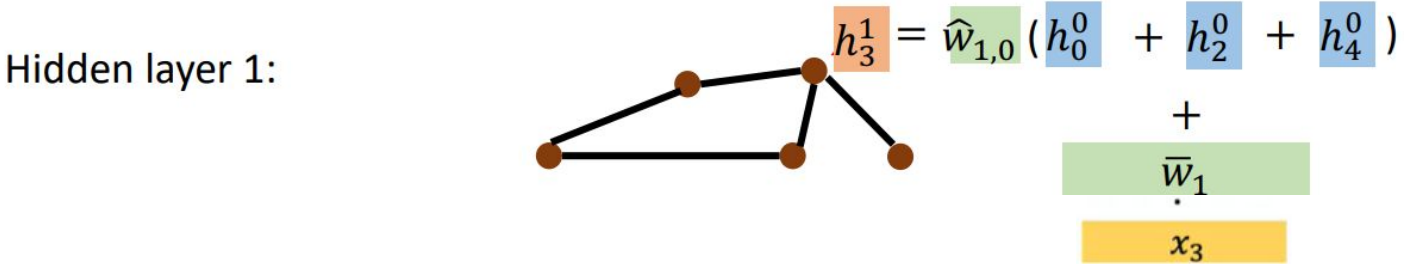


NN4G (Neural Networks for Graph)

https://ieeexplore.ieee.org/document/4773279

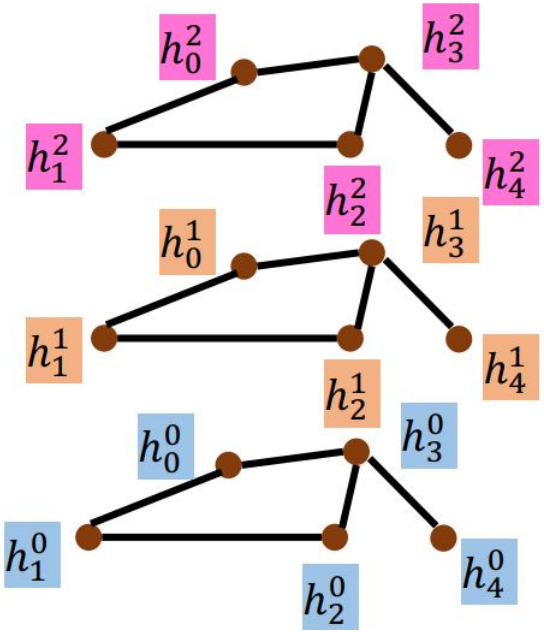






NN4G (Neural Networks for Graph)

Readout:



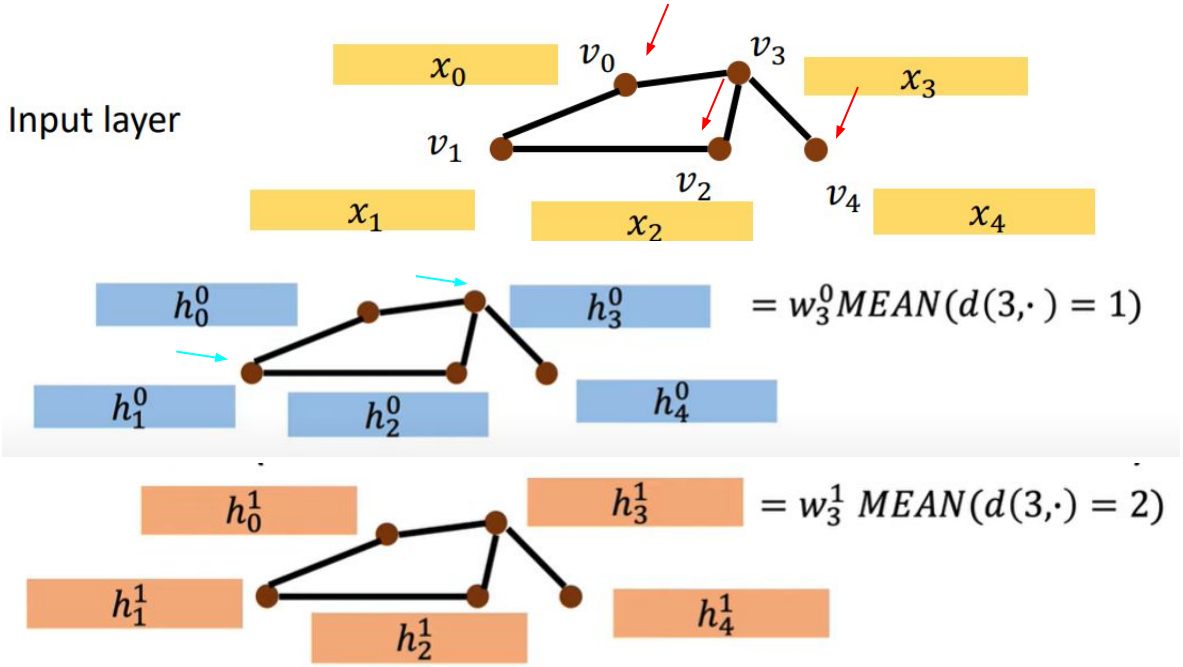
$$X_2 = MEAN(\,h^2\,) \xrightarrow{w_2}$$

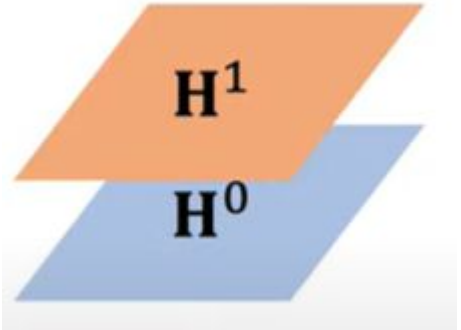
$$X_1 = MEAN(\,h^1\,) \xrightarrow{w_1} (+) \rightarrow y$$

$$X_0 = MEAN(\,h^0\,) \xrightarrow{w_0}$$

DCNN (Diffusion-Convolution Neural Network)

https://arxiv.org/abs/1511.02136





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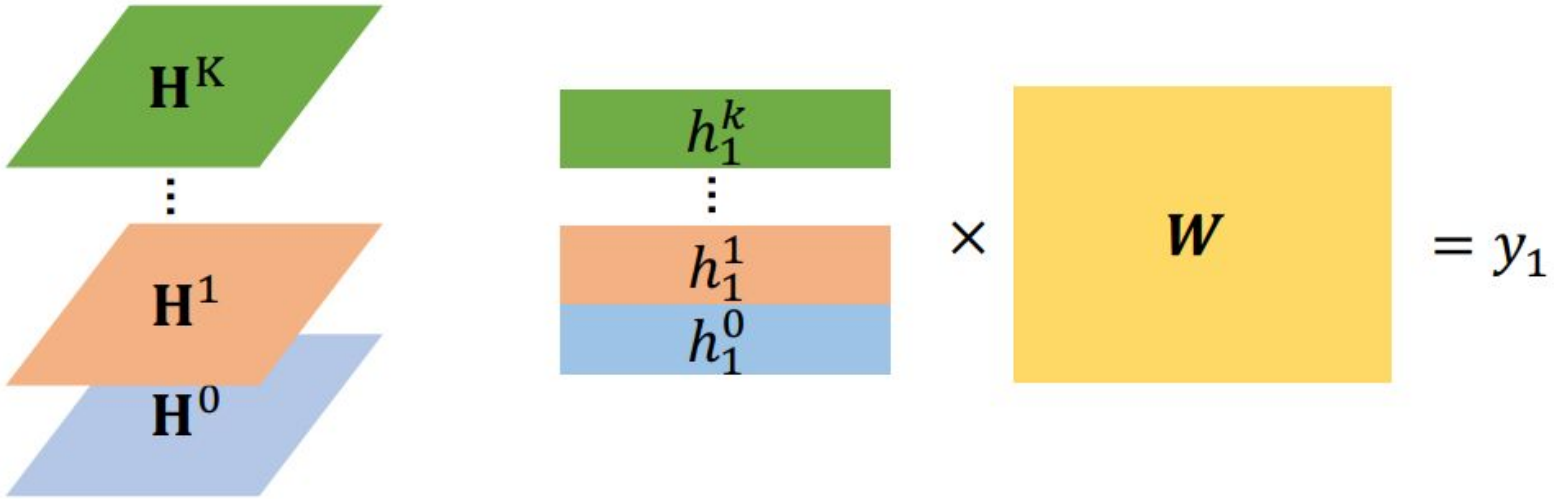

Python Library

Pytorch geometric

https://github.com/pyg-team/pytorch_geometric

Deep Graph Library

https://www.dgl.ai/