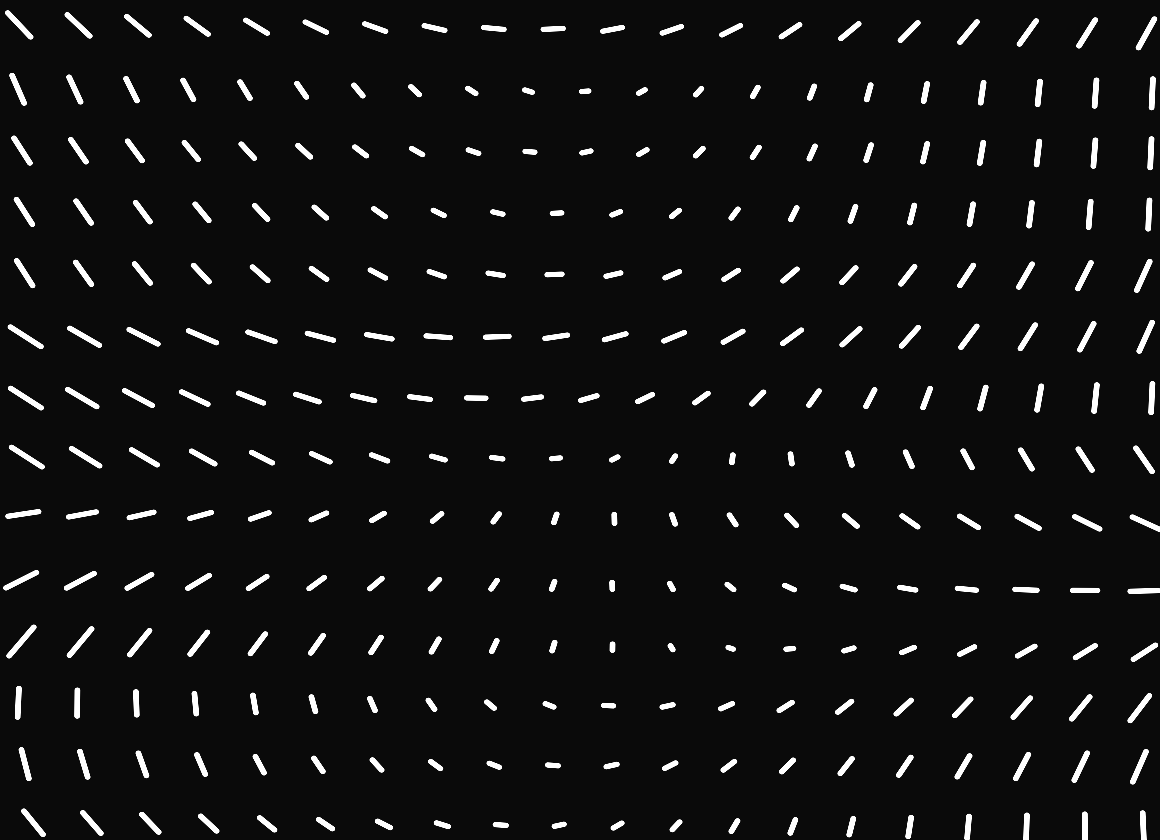


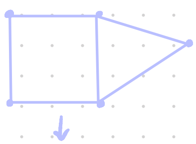
# Lecture #1

Graphs: Undirected, directed, weighted etc.

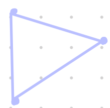
Mostly undirected graphs are used

Definition: $G = (V, E)$ $V$ = set of Nodes, $E$ = set of Edges

Properties of undirected graph adjency mat. nice.



G



subgraph of G

n-clique ⇒ fully connected graph size n.

spatial location not important in graph (in general)

In Geometric graph, the spatial location matters.

Point Cloud - Example of Geometric graph

Knowledge Graphs:

Nodes → Entities

Edges → Relationship betn entities

KG is a heterogenous graph.

KG completion popular area of research

# Lecture #2

## Why graph?

Graphs are general language for describing and analyzing entities with relations / interactions

Molecular sub graphs / community detection

Scene graphs → Image Segmentation

↳ Used in search engine, query graphs

Code Graphs → Bug detection

3D - meshes : Triangulations without intersections / Not Regular Graph

Triangles usually considered as it tells the Geometry of data (Topological data analysis)

CNNs for Graphs - first attempt only for Geometric Graphs

Challenges with Graphs:

- No spatial locality like Grid
- Arbitrary size and complex topological structure
- No fixed Node ordering

We need a model that permutation invariant.

Not very to compare two graphs

Learning a network (Graph Representation Learning): $f: u \rightarrow \mathbb{R}^d$
↳ Learn this

Thumb Rules:

Node-level Task → one Graph

Edge-level Task / Link prediction → one graph

Graph level prediction: Multiple Graph

community level: one Graphs

Tasks for KGs

- Link prediction / Triple Classification

Correspondence Problem in images: Difficult Tasks

Recommendation in E-community

Drug Repurposing

Polypharmacy side effect

Traffic Prediction using GNNs

Question Answering

Information Retrieval: PageRank

Reasoning on Reasoning

# Lecture # 3

## Graph Theory Basics

$G = (V, E)$

$G \rightarrow$ Graphs

$V \rightarrow$ Vertices, Nodes, points

$E \rightarrow$ Edges, lines, Arcs

parameter : $n = |V|$, $m = |E|$

## Graph Representation

Adj. Matrix

$A_{i,i} = 0$, $A = \begin{bmatrix} 0 & & & \\ & 0 & & \\ & & \ddots & \\ & & & 0 \end{bmatrix}_{n \times n}$

$n = |V|$

no. self loops

symmetric matrix.

Incidence matrix :

$$\begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{ccc} AB & BC & CA \end{array} \\ \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \end{array}$$

Incidence matrix can be generalized to K-cliques

Adj. List

edge list: AB AC AD

Node list:

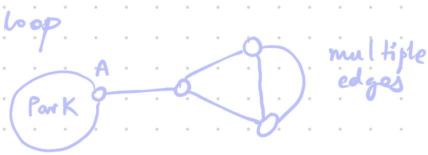
A → B C D
B → C, D
C → A B D
D → AB CE
E → D

weighted graph: AB – 2.5
AC – 1.5
CD – 3.0

$V = V(G) = \{A, B, C, \dots\}$

$E = E(G) = \{AB, BC, \dots\}$

Simple Graphs: No self loops
No multiple edges



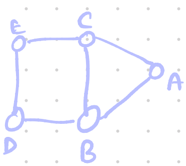

Degree: No. of nodes/edges connected to a node

$D(v)$, $deg(v)$

$deg(v) \leq n-1$

$ngh(v)$ or $N(v)$ → set of vertices in the neighbourhood of the node.

Example:




$n = |V| = 5$

$m = |E| = 6$

$V(G) = \{A, B, C, D, E\}$

$N(A) = \{B, C\}$

$N(B) = \{A, C, D\}$

$deg(v) = |N(v)|$

$deg(v) = 0$, isolated vertex

$deg(v) = 1$, pendant vertex

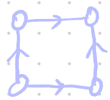
Null Graphs : no nodes, no edges

Empty Graphs : nodes but no edges

simple Graphs : $\sum_i deg(v_i) = 2|E|$, undirected

Directed Graphs :

$AB \neq BA$

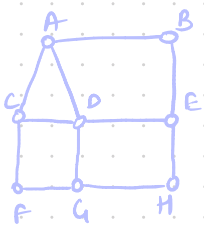


ordered pair of vertices

In degree : $deg^-(v)$

Out degree : $deg^+(v)$

Degree sequence : 2, 2, 2, 3, 3, 4, ...




Eccentricity (V) : max distance from any vertex

$e(A) = 3$

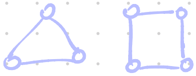
Radius of Graph

$r(G) =$ minimum eccentricity of any vertex in a graph

for a disconnected Graph,

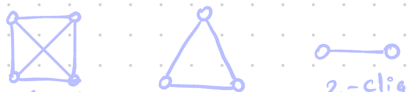
radius $= \infty$.

K-Regular Graphs : All nodes having same degree K.



2-regular Graphs

Complete Graphs : All nodes connected to each other



4-clique 3-clique 2-clique

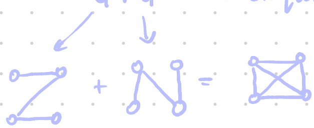
Cycle Graphs : $n \geq 3$, every edge form cycle of length $n$.

2-regular Graphs always cycle graphs

Complement of Graph : Graph $G'$ that is obtained by toggling all the edges

i.e. $uv \in E(G')$ iff $uv \in E(G)$

$G + G' \longrightarrow$ n-clique



Path Graphs : removing one edge from cycle Graphs will give path Graph.

H is a sub Graph of G

$V(H) \subseteq V(G)$ , $E(H) \subseteq E(G)$

Bipartite Graph : $V = L \cup R$ , L & R are independent sets

Independent set : $S \subseteq V(G)$ s.t. for any $u, v \in S$, $uv \notin E(G)$

K-partite Graph : divide Graph into K independent sets

walk : A sequence a adjacent vertex

Trail : All edges distinct

Path : All nodes are distinct

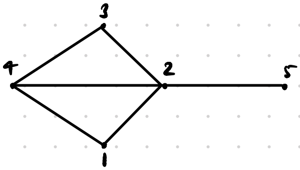
cycle : closed path

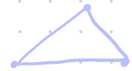
# Lecture #4

WL-Test → Graph Isomorphie

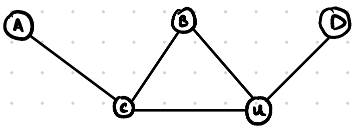
# Lecture #5

$\beta = 0.5$ $\quad \beta A_{1,3}$

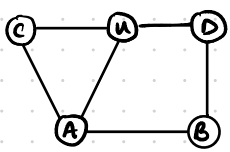


$$c = \begin{bmatrix} 0.4119 \\ 0.582 \\ 0.4119 \\ 0.523 \\ 0.216 \end{bmatrix} \begin{matrix} \\ \to 1 \\ \\ \to 2 \\ \to 5 \end{matrix} \qquad \lambda = (2.68, -1.27, 0.33, 0.00)$$




| 0 | 1 | 2 | 3 |
|---|---|---|---|
| u − B | u − C − A | D − u − C | B − u − C |
| u − C | | D − u − B | |
| u − D | | | |
| 3 | 1 | 2 | 1 |




$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \beta \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}$$

| 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|
| 3 | u − A − B | | | | |
| u − C | | | | | |
| u − A | | | | | |
| u − D | | | | | |

$$\text{Katz} = (I - \beta A)^{-1} - I$$

# Lecture #6

We want Graph embedding

$K(G, G') = f_G^T f_{G'}^T$

Normalize $f_G \longrightarrow h_G = \frac{f_G}{sum(f_G)}$

$K(G, G') = h_G^T h_{G'}$

WL - Kernel $\longrightarrow$ WL - Isomorphism

considering only those pairs that co-occur in the

Random walk $\longrightarrow$ similar to words in sentence

Word2Vec
doc2Vec
Par2Vec

DeepWalk
Node2Vec

# Lecture #7

$$\begin{matrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{matrix} \longrightarrow \begin{matrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{matrix}$$

# Lecture #8

$-1 = e$

$$P\{|D^{l} - D^{m}| \geq \varepsilon\} < \delta$$

$$2n\left[\frac{\pi}{2} - \sin^{-1}\left(\frac{k}{2n}\right)\right]$$

$$m = \left[\frac{2}{\varepsilon^2}\right.$$

$$n\pi - 2n\sin^{-1}\left(\frac{k}{2n}\right)$$

$$Re\left(e^{i2n\cos^{-1}\left(\frac{k}{2n}\right)}\right)$$

$$\sum_{k=0}^{2n} (-1)^k \binom{2n}{k} \cos\left(2n\cos^{-1}\left(\frac{k}{2n}\right)\right)$$

$$e^{n\pi i}$$

$$(-1)^k \binom{2n}{k}$$

$$Re\left[\sum_{k=0}^{2n} \binom{2n}{k} e^{i2n\cos^{-1}\left(\frac{k}{2n}\right) + k\pi i}\right.$$

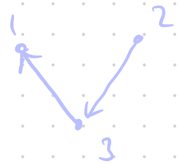
$$\Downarrow$$

$$\left.x^{2n-k} y^{k}\right]\Big)$$

$$Re\left[(x+y)^{2n}\right)$$

$$\cos^{-1}\left(\frac{k}{2n}\right)$$

# Lecture #9




$$\begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{vmatrix}^T$$

# Lecture #11

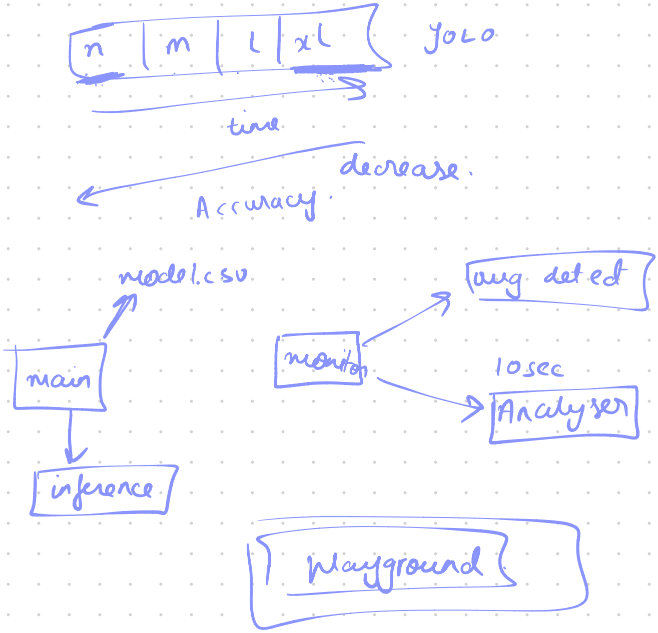
$D^{-1/2} \hat{A} D^{1/2}$

## Design space of GNNs — Important

In practice, 1, 2 or max 3 layers of GNNs

Questions: 1) GraphSAGE How does it work?

2) Project: Is beating the baselines enough?


n | m | l | xl
YOLO
time
decrease.
Accuracy.
model.csv
main
inference
monitor
avg detect
10sec
Analyser
playground

# Lecture #12

$\begin{pmatrix} 2 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 4 \end{pmatrix}$

# Lecture #14

# Lecture #15