## Notations and definitions

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## 1 Notations

- 1. Graph  $\mathcal{G}(\mathcal{V}, \mathcal{E})$  represents a collection of nodes  $\mathcal{V}$ , interconnected by a set of edges  $\mathcal{E}$ . The number of nodes  $|\mathcal{V}| = n$  and the number of edges  $|\mathcal{E}| = m$ .
- 2. Edgeset  $\mathcal{E} = \{e_1, \dots, e_m\}$  where the *i*-th edge,  $e_i = (u, v); u, v \in \mathcal{V}$ . Each edge can either be directed or undirected.
- 3. Adjacency matrix **A** is used to represent a graph.  $\mathbf{A}_{u,v} = \mathbb{1}[u \text{ and } v \text{ are connected}].$
- 4. Subgraph  $\mathcal{S}(\mathcal{V}_{\mathcal{S}}, \mathcal{E}_{\mathcal{S}})$  is a subgraph of  $\mathcal{G}$ , where  $\mathcal{V}_{\mathcal{S}} \subseteq \mathcal{V}$  and  $\mathcal{E}_{\mathcal{S}} \subseteq \mathcal{E}$ .
- 5. Node feature  $x_v \in \mathbb{R}^d$  describes the attributes of node v. Node feature matrix  $X \in \mathbb{R}^{n \times d}$ .
- 6. Edge feature  $x_{u,v}^e \in \mathbb{R}^d$  descibes the attributes of the edge (u,v). Edge feature matrix  $X^c \in \mathbb{R}^{m \times c}$ .
- 7. Label is a target associated with either a node  $Y_v$ , an edge  $Y_{u,v}$ , a subgraph  $Y_S$ , or a graph  $Y_G$ .

## 2 Definitions

**Walk** A walk of length l from node  $v_1$  to  $v_l$  is a sequence of nodes and edges  $v_1 \xrightarrow{(v_1, v_2)} v_2 \xrightarrow{(v_2, v_3)} \dots \xrightarrow{(v_{l-2}, v_{l-1})} v_{l-1} \xrightarrow{(v_{l-1}, v_l)} v_l$ .

Path A walk with all distinct nodes.

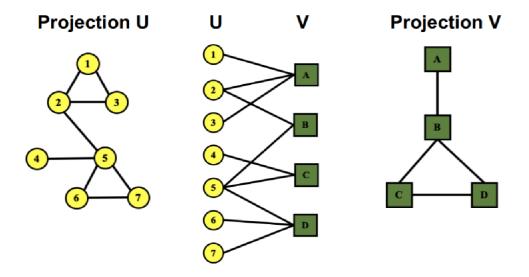


Figure 1: Example of a bipartite graph and the projections of the independent sets U and V (Source: CS224W)

**Distance** Distance dist(u,v) is the length of the shortest path between nodes u and v.

**Diameter** Longest distance among all pairs of nodes in the graph.

**Bipartite graph** A graph whose nodes can be divided into two disjoint sets U and V such that every edge can only connect a node in U to one in V, i.e, U and V are independent sets. Figure 1 illustrates an example of a bipartite graph.

**Neighborhood** For a node v, its neighborhood  $\mathcal{N}(v)$  is the collection of nodes that are connected to v.

k-hop neighborhood is the set of all the nodes that are k hops away from node v:  $\mathcal{N}^k(v) = \{u|dist(u,v) = k\}$ 

Clustering coefficient For a node v, it measures how connected the nodes of  $\mathcal{N}(v)$  are to one another. Formally,  $e_v = \frac{\#(\text{edges among the nodes of } \mathcal{N}(v))}{\binom{deg(v)}{2}}$  Figure 2 gives examples.

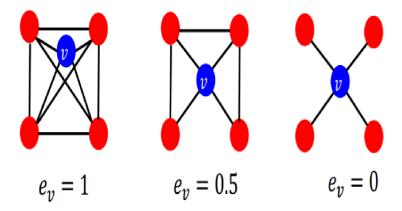


Figure 2: Examples of clustering coefficient of graphs (Source: CS224W)