DSC40B: Theoretical Foundations of Data Science II

Lecture 10: *Graphs: basics and representations*

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Graphs: directed and undirected

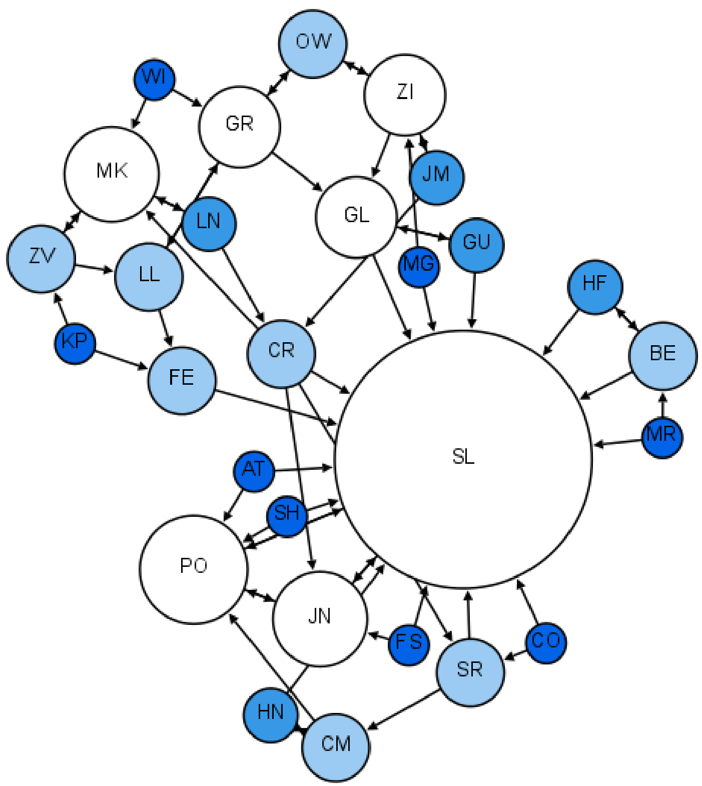
Common data types

- A set of feature vectors in some feature space (e.g, R^d)
  - A collection of patients' record, each represented by a feature vector containing information such as name, age, health history etc.
  - Focus on attributes of individuals

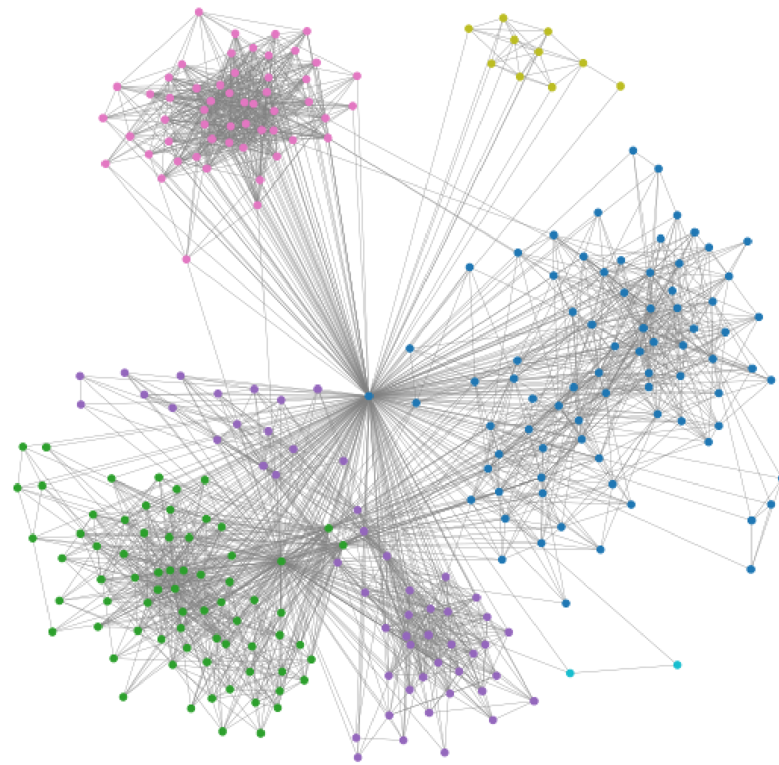
- Graph data:
  - Focus on (pairwise) relations among individuals
  - Social networks, co-authorship networks, knowledge graphs

Examples

- Social networks



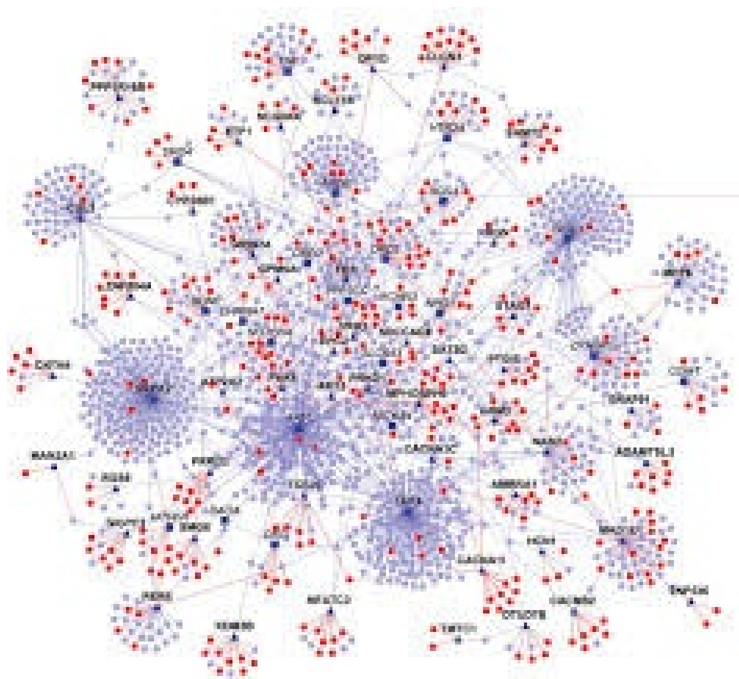
Moreno's sociogram of a 2nd grade class



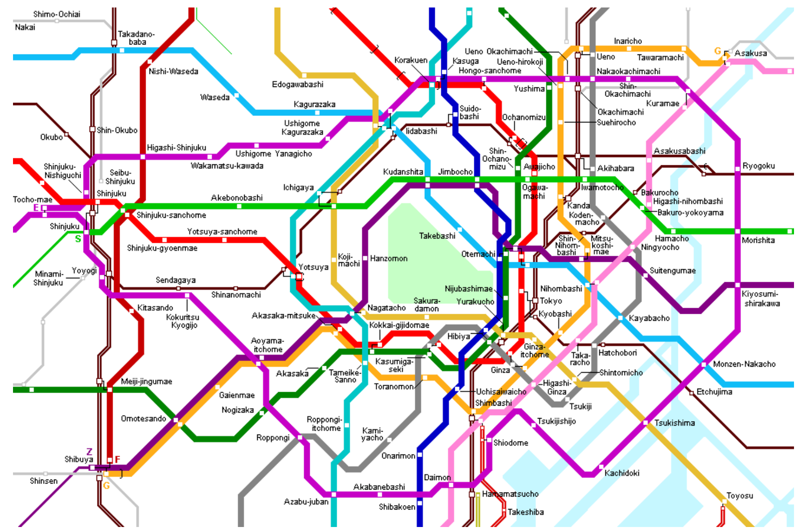
Facebook friendship social graph

Examples

- Biological networks
- Road networks



Protein-protein interaction networks



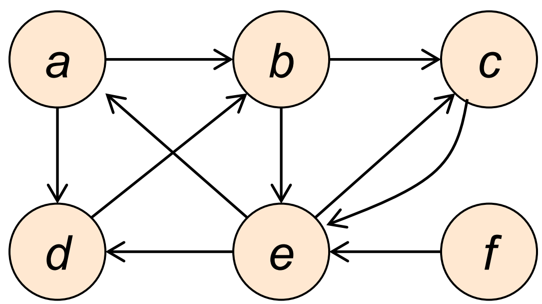
Tokyo subway map

What is a graph?

- On the high level, a graph G is a pair $G = (V, E)$
  - V: a set of graph nodes (or vertices)
  - $E \subset V \times V$: a set of graph edges
    - each edge $(a, b) \in E$ represents a certain relation between the pair of graph nodes $a, b \in V$
- Directed vs undirected graphs

Directed graphs

- A directed graph (or digraph) G is a pair (V, E) where V is a finite set of nodes and E is a set of *ordered pairs* called (directed) edges.



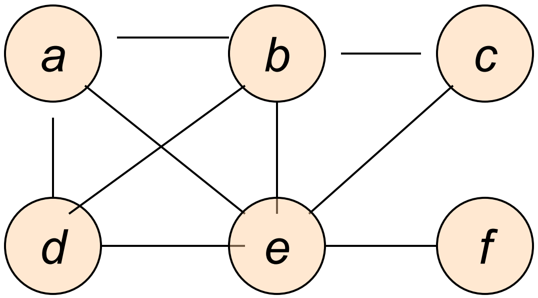
- $G = (V, E)$ where
  - $V = \{a, b, c, d, e, f\}$;
  - $E = \{(a,b), (a,d), (b,c), (b,e), (c,e), (d,b), (e,a), (e,c), (e,d), (f,e)\}$

Remarks

- Note that each edge $(a, b) \in V \times V$ is an ordered pair
  - meaning that there is an edge from a to b
- Hence edges $(a, b) \neq (b, a)$
  - e.g, Alex follows Elon Musk in twitter, so (Alex, Elon) is an edge in E. But Elon does not follow Alex, so (Elon, Alex) $\notin E$
  - Note that both (a, b) and (b, a) could be in the edge set
- There can also be self-loop: (a, a)
- Simple graph:
  - for any ordered pair, there can be at most one edge in E

Directed graphs

- A undirected graph G is a pair (V, E) where V is a finite set of nodes and E is a set of *unordered pairs* called edges.



- $G = (V, E)$ where
  - $V = \{a, b, c, d, e, f\}$;
  - $E = \{(a, b), (a, d), (a, e), (b, c), (b, d), (b, e), (c, e), (d, e), (e, f)\}$

Remarks

- An edge is a subset of nodes V with cardinality 2.
  - Hence the formal way to represent an edge is $\{a, b\}$
  - By convention however, we often still write it as (a, b).

- There is no order for each pair
  - Thus edge $(a, b) = (b, a)$

- Simple graphs:
  - There is no self-loops of the form (a, a)
  - There is at most one edge for each pair of nodes $\{a, b\}$

Summary

- Edge direction ?
  - directed graph: Yes
  - undirected graph: No

- Self-loop?
  - directed graph: Yes
  - undirected graph: No

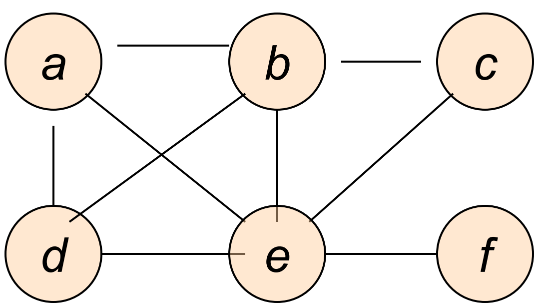
- Opposite edges: (a, b) and (b, a) ?
  - directed graph: Yes
  - undirected graph: No (they are the same edge)

Graphs: More notations

Node degree in undirected graph

- Given an undirected graph $G = (V, E)$
  - given an edge $e = (u, v) \in E$, we refer u, v as end-points of e
  - we say that edge e is incident on node u if u is an end-point of e

- Given an undirected graph $G = (V, E)$, the degree of a node $v \in V$ is
  - $\deg(v) :=$ number of edges incident on v



- Example:
  - $\deg(e) = 5, \ \ \deg(f) = 1$

Observations

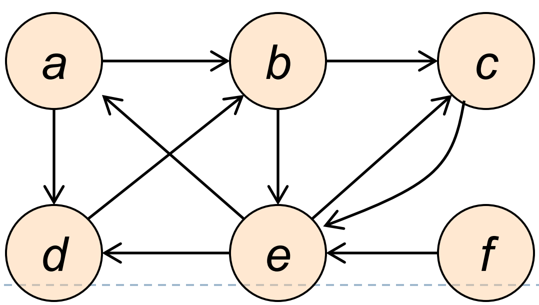
- Given a undirected graph $G = (V, E)$ with $n = |V|$
  - $0 \leq \deg(v) \leq n - 1$, for any node $v \in V$
  - $\sum_{v \in V} \deg(v) = 2|E|$

- Given a undirected graph $G = (V, E)$ with $n = |V|$
  - The maximum number of edges is $\frac{n(n-1)}{2}$
  - This also implies that $|E| = O(n^2)$

- A undirected graph $G = (V, E)$ is a complete graph iff
  - There is one edge between every pair of distinct nodes in V
  - i.e, $|E| = \frac{n(n-1)}{2}$

Node degree in directed graph

- Given a directed graph $G = (V, E)$, the in-degree of a node $v \in V$ is
  - $\text{indeg}(v) :=$ number of edges entering v
- Given a directed graph $G = (V, E)$, the out-degree of a node $v \in V$ is
  - $\text{outdeg}(v) :=$ number of edges leaving v
- Sometimes we use degree to denote the sum
  - $\deg(v) = indeg(v) + outdeg(v)$



- Example:
  - $\text{indeg}(e) = 3, \quad \text{outdeg}(e) = 3$
  - $\text{indeg}(f) = 0, \ \text{outdeg}(f) = 1$

Observations

- Given a directed graph $G = (V, E)$ with $n = |V|$
  - $0 \leq \mathrm{indeg}(v),\ \mathrm{outdeg}(v) \leq n$, for any node $v \in V$
  - $\sum_{v \in V} \mathrm{indeg}(v) = \sum_{v \in V} \mathrm{outdeg}(v) = |E|$

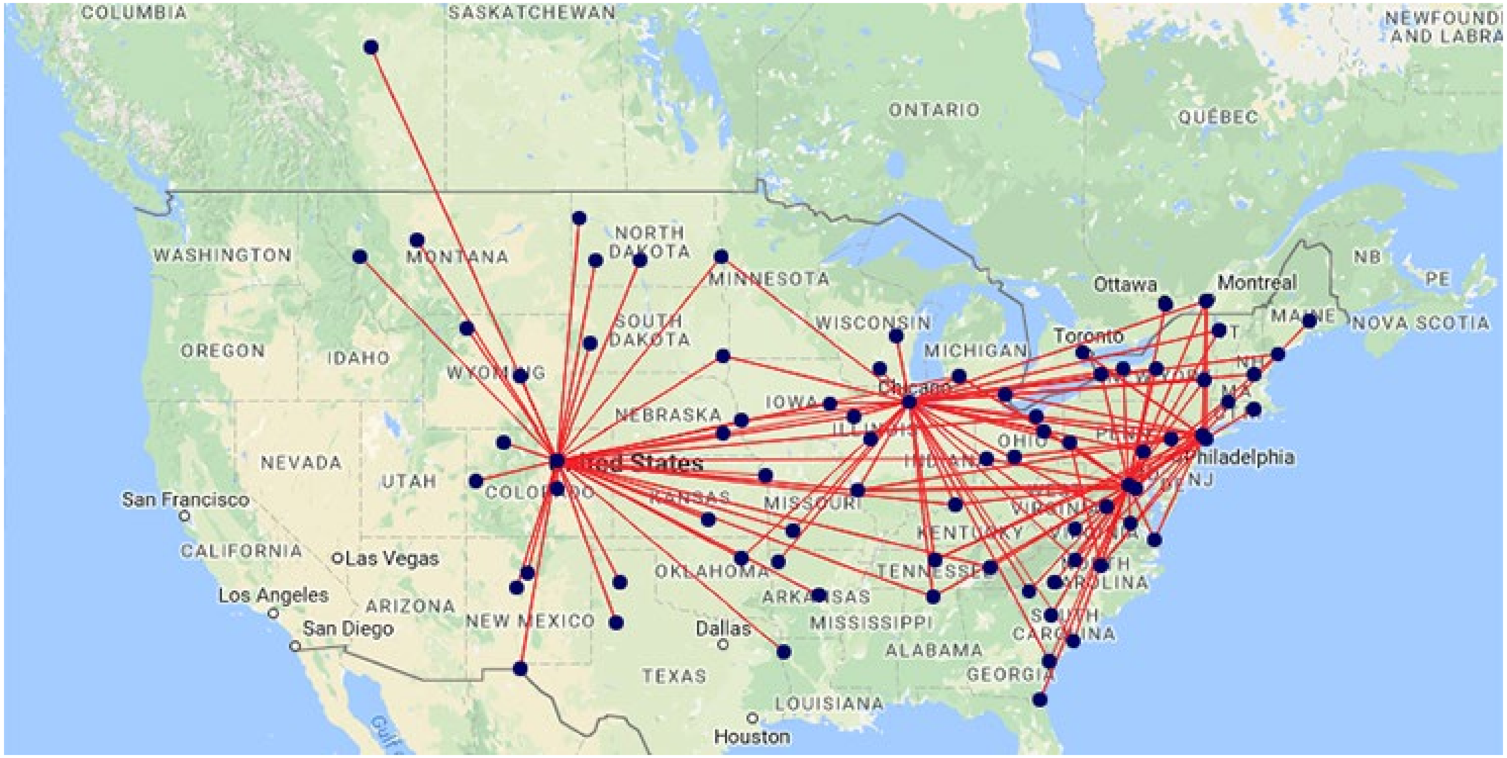
- Given a directed graph $G = (V, E)$ with $n = |V|$
  - The maximum number of edges is n^2
  - This also implies that $|E| = O(n^2)$

More notations

- Given a undirected graph $G = (V, E)$
  - the set of **neighbors** of $v \in V$ is the set of all nodes in V that share an edge with v
- Given a directed graph $G = (V, E)$
  - the set of **successors** of $v \in V$ is the set of all nodes at the end of an edge leaving v
  - the set of **predecessors** of $v \in V$ is the set of all nodes at the start of an edge entering v
- By convention, for a directed graph
  - the set of **neighbors** of a node often refers to the set of successors of this node.

Paths, reachability and connectivity

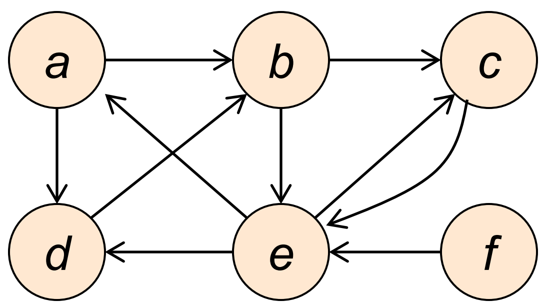
Example



Can we fly from Columbus, Ohio to Denver, Colorado?

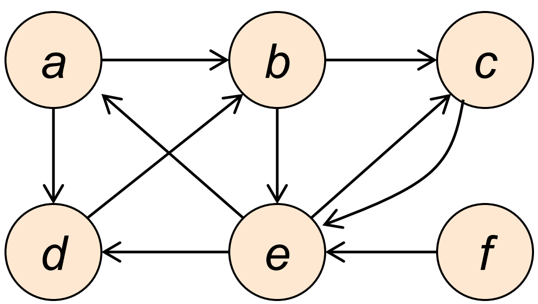
Paths

- A path from u to u' in a (directed or undirected) graph G = (V, E) is a sequence of one or more nodes $u = v_0, v_1, \ldots, v_k = u'$ such that there is an edge between each consecutive pair of nodes in the sequence.



Paths

- The length of a path = # of nodes −1 = # of edges in a path
  - The length of a path could be 0
- A path is simple if it visits each node only once
  - In this class, we usually consider only simple paths.
- A cycle is a path where the first and last nodes are the same

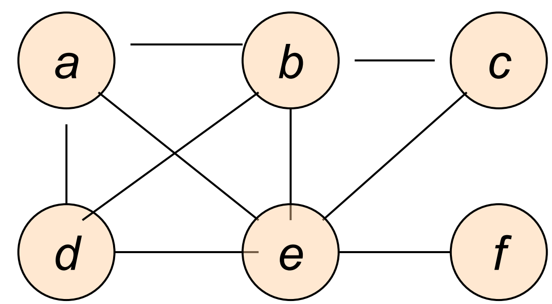


Reachability

- Node u is reachable from node v if there is a path from v to u

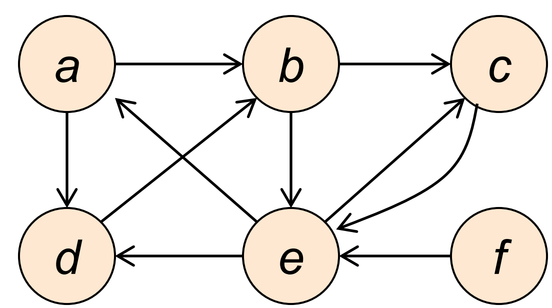
- In undirected graph,
  - If u is reachable from v, then v is reachable from u

G_1



- In a directed graph
  - u is reachable from v does not imply that v is necessarily reachable from u
  - Reachability is not symmetric for directed graphs!

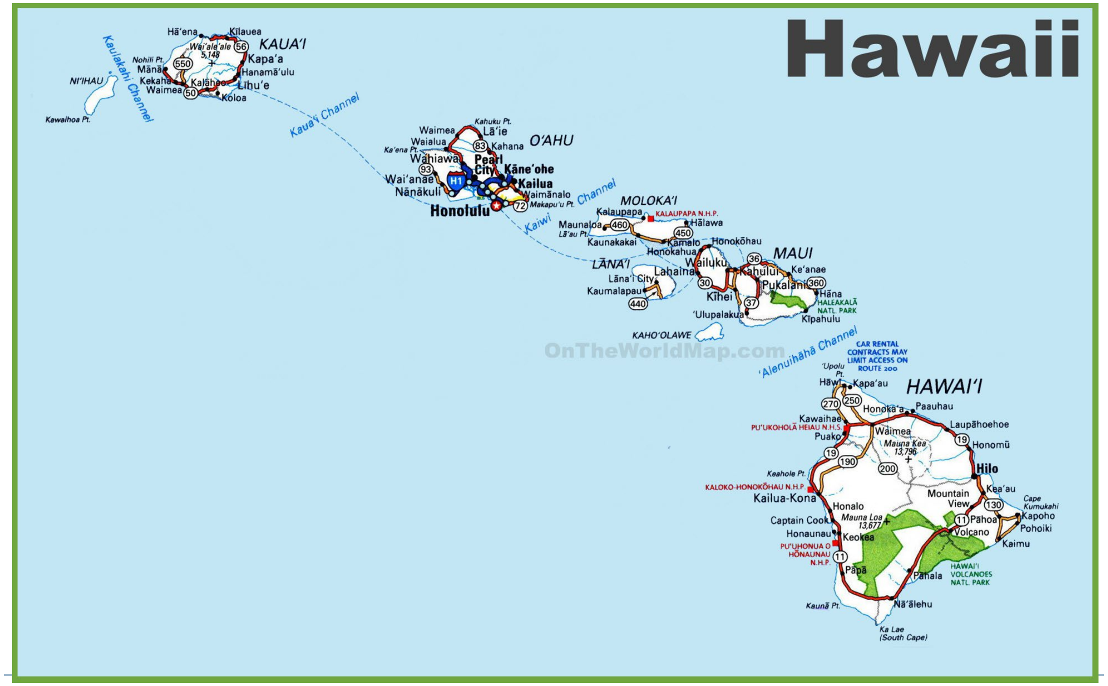
G_2



Connectivity

- This concept is for undirected graphs.
- A undirected graph is connected if every node is reachable from every other node. Otherwise, it is disconnected.

A graph is disconnected means that there exists at least one pair of nodes u, v such that u is not reachable from v.



Connected components

- A connected component of a graph $G = (V, E)$ is a maximally-connected subset of nodes of V.

- That is, given a undirected graph $G = (V, E)$, a connected component is a set $C \subseteq V$ such that
  - any pairs $u, v \in C$ are reachable from one another; and
  - if $u \in C$ and $z \notin C$, then u and z are not reachable from one another.

- If a undirected graph is connected, then it has only one connected component.

- For directed graphs, there is a concept called strongly connected components.

Representations of graphs

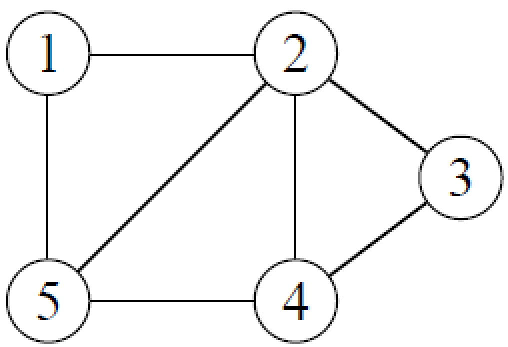
Representation of graphs

- How do we represent a graph in the computer
  - e.g, to be used as input to an algorithm

- Three representations
  - Adjacency matrix
  - Adjacency list
  - Dictionary set

Adjacency matrix representation

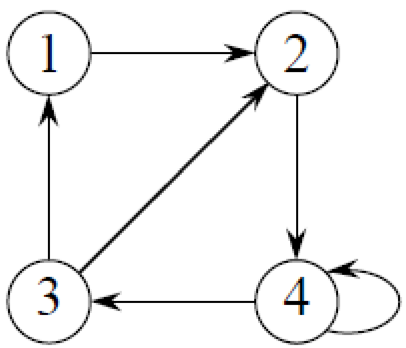
- Assume $V = \{v_0, v_1, \dots, v_{n-1}\}$ with $n = |V|$
- Adjacency matrix of a graph is a $n \times n$ matrix adj
  - adj$[i, j] = \begin{cases} 1, & (v_i, v_j) \in E \\ 0, & otherwise \end{cases}$



	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

Adjacency matrix representation

- Assume $V = \{v_0, v_1, \ldots, v_{n-1}\}$ with $n = |V|$
- Adjacency matrix of a graph is a $n \times n$ matrix adj
  - $\text{adj}[i,j] = \begin{cases} 1, & (v_i, v_j) \in E \\ 0, & otherwise \end{cases}$



$$\begin{array}{c|cccc|} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 & 1 \\ 3 & 1 & 1 & 0 & 0 \\ 4 & 0 & 0 & 1 & 1 \\ \hline \end{array}$$

Observation:
- If the graph is undirected, then this matrix is a symmetric matrix
- If the graph is directed, then the adjacency matrix is not necessarily symmetric

Complexity

- Size of Adjacency matrix
  - $\Theta(|V|^2)$
- Time complexity of operations
  - Edge query:
    - is the edge $(v_i, v_j) \in E$?
  - Degree query:
    - What is the degree of vertex v_i ?

operation	code	time
edge query	`adj[i,j] == 1`	$\Theta(1)$
degree(i)	`np.sum(adj[i,:])`	$\Theta(\|V\|)$

Remarks

- Pros:
  - Support very efficient edge queries
  - Simple and easy to use
    - only need to allocate a $|V| \times |V|$ (Numpy) array
  - Easy to manipulate via linear algebra
    - e.g, (i,j)-th entry of A^2 gives number of hops of length 2 between v_i and v_j

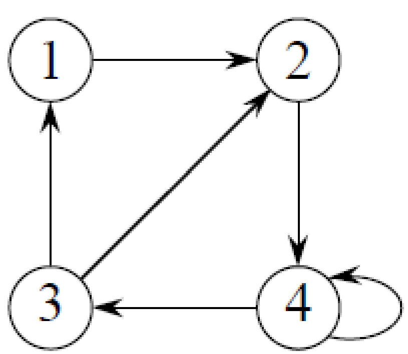
- Cons:
  - Take $\Theta(|V|^2)$ no matter what the graph looks like
  - In real-life, graphs are often sparse, with far fewer number of edges
    - e.g, facebook has 2.7 billion users
      - $|V|^2 = (2.7 \times 10^9)^2 \approx 7.3 \times 10^{18}$ bits

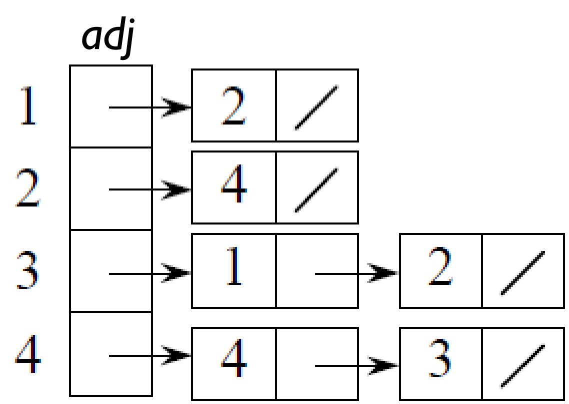
        ≈ 11862 years of video at 1080p

        ≈ 109 copies of the internet as it was in 2000

Adjacency list representation

- Adjacency matrix allocates a bit for each $|V|^2$ potential edge
  - What if we only store the edges in the graph?
- Adjacency lists
  - Each vertex *u* has a list, recording its neighbors
    - i.e., all *v*'s such that $(u, v) \in E$
  - An array of $|V|$ lists
    - *adj[i].size* = size of AdjList for node v_i
    - *adj[i]* = adjacency list for node v_i





Size complexity

- For each vertex v_i, its adjacency list $\text{adj}[i]$ has size =
  - $\deg(v_i)$ if the graph is undirected
  - $\text{outdeg}(v_i)$ if the graph is directed
- Hence each edge will be stored
  - twice in the adjacency list if the graph is undirected
  - once if the graph is directed
- Total size:
  - $\Theta(|V| + |E|)$
  - where $\Theta(|V|)$ for the outer array, and $\Theta(|E|)$ for the total lengths of inner lists .

Time complexity

- Time complexity of operations
  - Accessing the list of neighbors for a specific vertex v_i
    - takes $\Theta(1)$ time, as just return the list $adj[i]$
  - edge query: is edge $\left(v_i, v_j\right) \in E$?
    - takes $\Theta(length\ of\ adj[i]) = \Theta(\deg(v_i)) = O(|V|)$
      - (deg should be out-deg for directed graphs)
  - degree query: what is the **degree** of v_i (in undirected graph), or what is the **outdegree** of v_i (in directed graph)
    - takes $\Theta(1)$ time
    - **However,** for directed graph, checking **indegree** takes $O(|V| + |E|)$ time!

- Summary of time complexity:
  - Note: below "degree" refers to the "**degree**" of a node for an undirected graph, but "**out-degree**" of a node for a directed graph!

operation	code	time
edge query	`j in adj[i]`	$\Theta(\text{degree}(i))$
degree(i)	`len(adj[i])`	$\Theta(1)$

Remarks

- Pros:
  - Optimal space complexity
    - $\Theta(|V| + |E|)$ is the least possible (asymptotically), thus space complexity is optimal
  - Fast for (out-)degree queries.

- Cons:
  - Slow for edge queries
  - No linear algebra operations such as A^2

- Adjacency matrix:
  - Fast edge queries, potentially large space

- Adjacency list:
  - Slow edge queries, but efficient in space

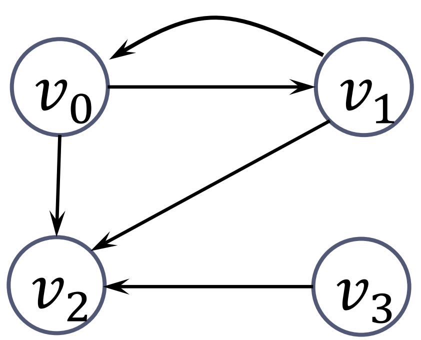
Can we take the advantage of both?

Dictionary-set representation

- Idea:
  - why not changing the inner list to a Hash table to store the list of neighbors (i.e, adjacency list) of each node
    - E.g, using the Set data structure in python.
  - this will make membership query (which is essentially what edge query is about) efficient!
    - to check whether (v_i, v_j) is in E, we just need to check whether v_j is in the adjacency list of v_i, which is a membership query in the $\mathrm{adj}[i]$
  - We further change the outer array to also a Hash table
    - e. g, using the dict data structure in python
    - this also allows us to map non-integer indexed nodes

Dictionary-of-set implementation

- Dictionary-of-set implementation
  - Using an outer hash table (dict) to represent all non-empty adjacency list for all nodes
  - For each node with non-zero neighbors, using a hash table (set) to store all its neighbors



Complexity

- Space complexity
  - $\Theta(|V| + |E|)$

- Time complexity (in expectation)

operation	code	time
edge query	`j in adj[i]`	$\Theta(1)$ average
degree(i)	`len(adj[i])`	$\Theta(1)$ average

- However,
  - note that time complexity is average time, and also there will be overhead of using Hash tables.

Dictionary-of-set implementation

- On datahub:
  - import dsc40graph
- Or download from the course page.

FIN