Graph Theory and Algorithms

Traversal, Toposort, Shortest Path, Max Flow, Spanning Tree

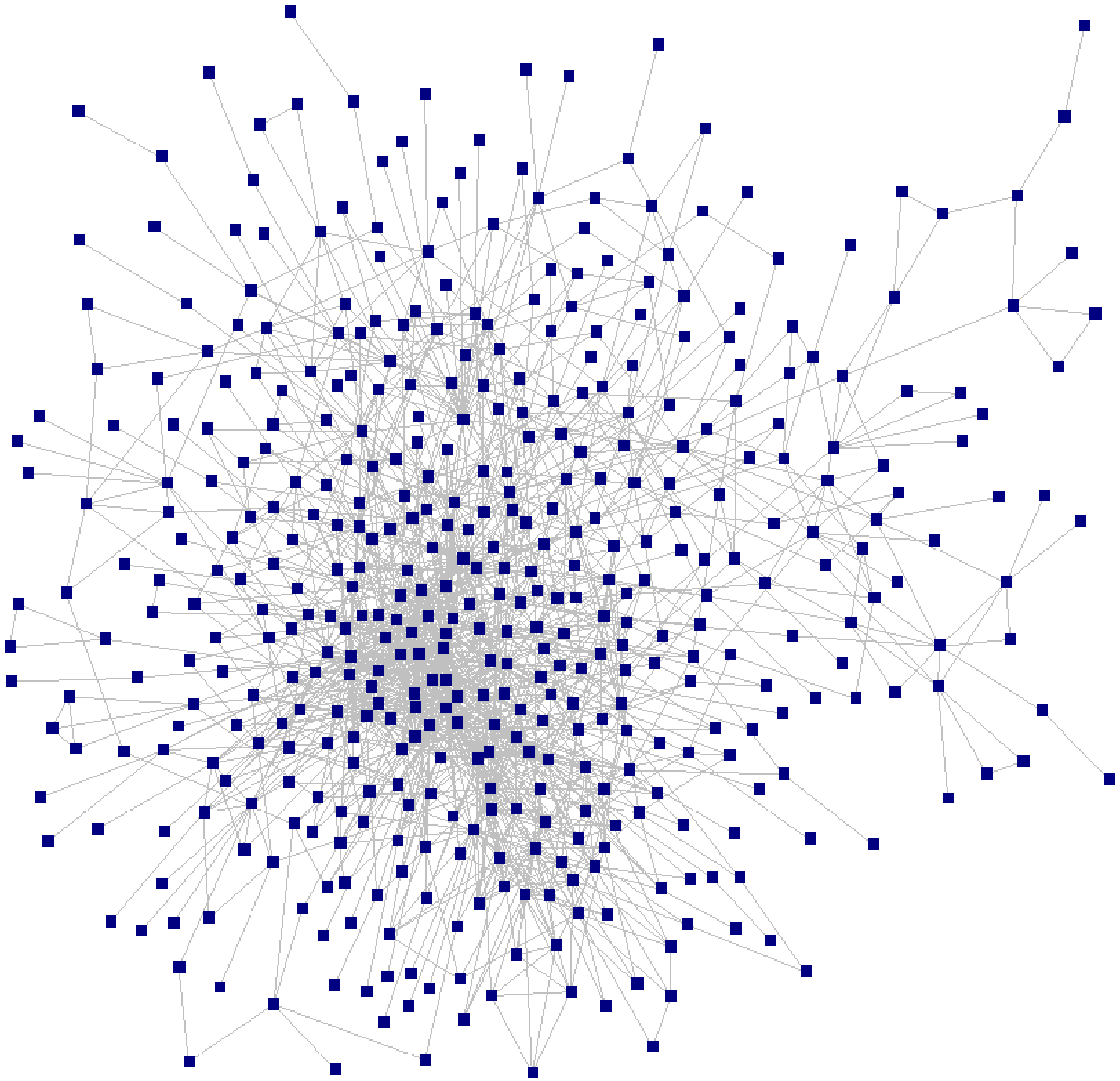
Prof. Karl Ezra Pilario, Ph.D.

Process Systems Engineering Laboratory
Department of Chemical Engineering
University of the Philippines Diliman

What is a graph?

A collection of nodes and edges.

Examples:	Node	Edge
Social networks	Person	Friendship
Contagions	Person	Contact
Country map	City	Roads
Chemical plant	Equipment	Piping
Reaction network	Compound	Reaction
Power grid	Sources/loads	Power lines



Source: http://www.orgnet.com/Erdos.html

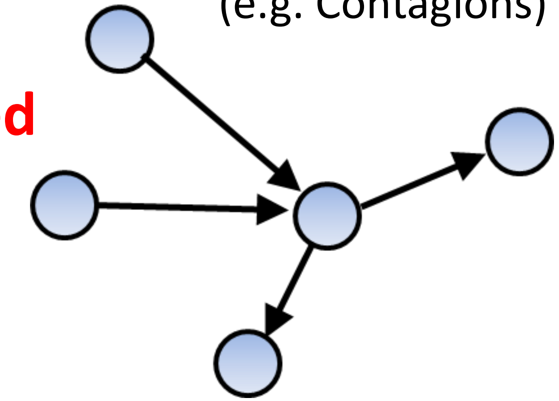
Graph Terminologies

Different kinds of graphs:

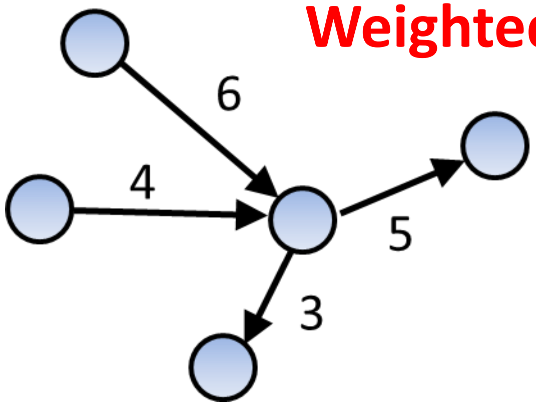
Directed graph

(e.g. Contagions)

Unweighted



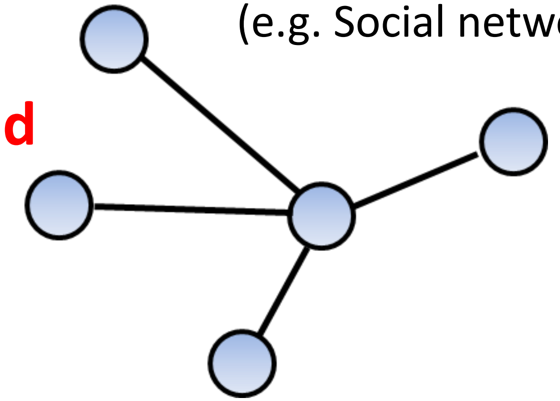
Weighted



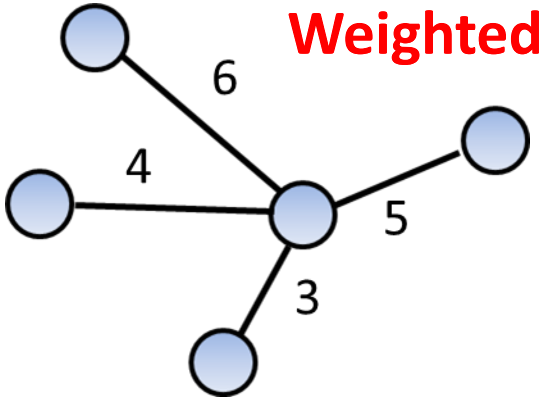
Undirected graph

(e.g. Social networks)

Unweighted



Weighted

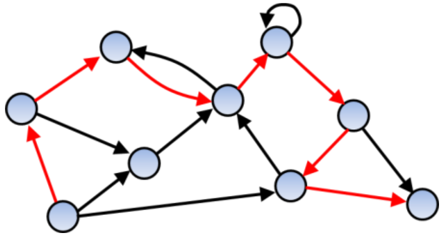


Graph Terminologies

Other definitions:

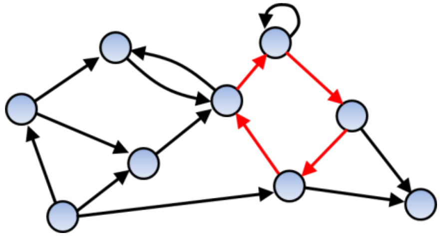
Path

An ordered sequence of nodes connected by edges.



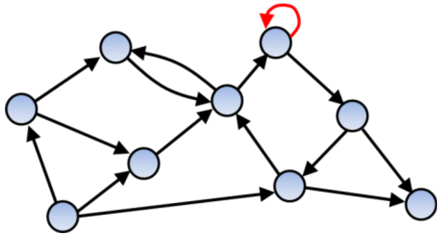
Cycle

A path with the same start and end node.



Self-loop

An edge connecting a node to itself.



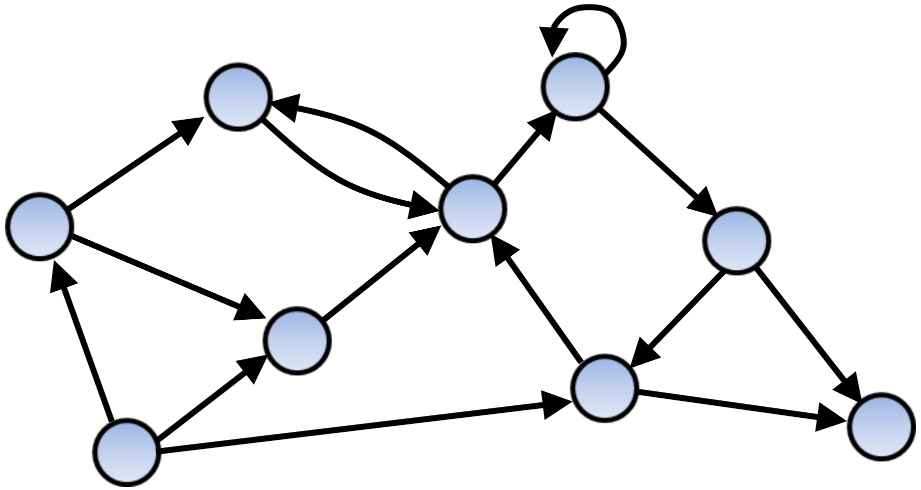
A self-loop is a *cycle of length 1*.

A path in which *all nodes are distinct*, except possibly the start and end nodes, is called a *simple path*.

A simple path with the same start and end node is a *simple cycle*.

Any graph with no self-loop is called a *simple graph*.

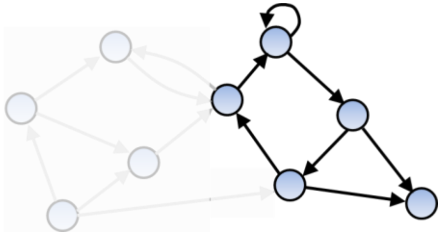
A digraph no cycles is called a *DAG (directed acyclic graph)*.



A directed graph (digraph)

Subgraph

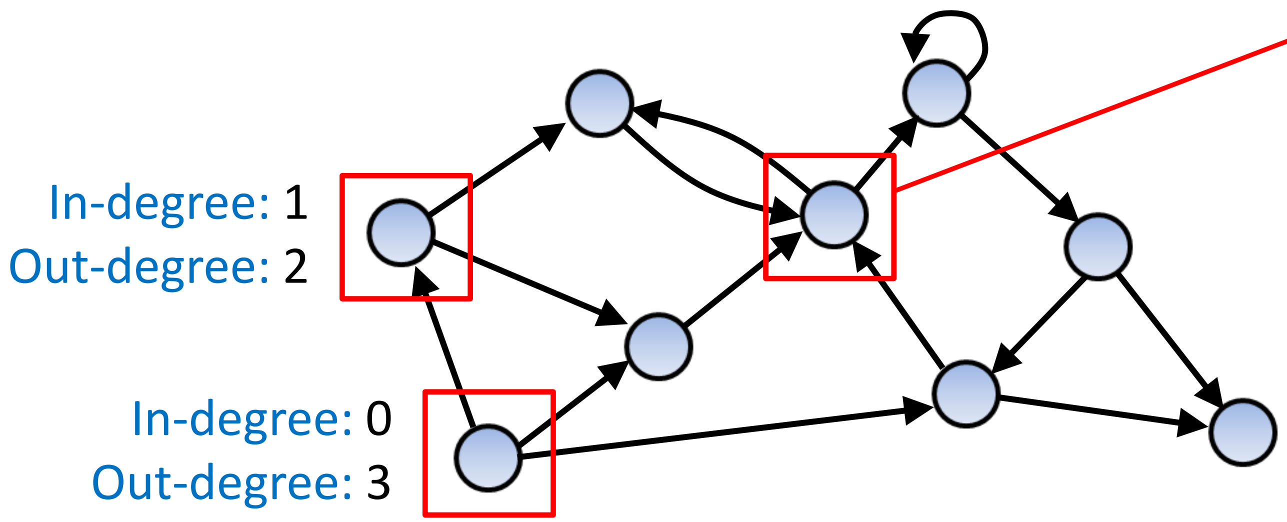
A graph containing only a subset of the edges and nodes of the original graph.



Graph Terminologies

Other definitions:

A directed graph (digraph)



In-degree: 3
No. of edges entering it.

Out-degree: 2
No. of edges leaving it.

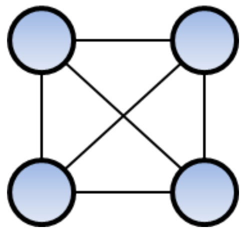
For an undirected graph, the in-degree and out-degree are the same. Hence, they are simply called *degree*.

Complete graph

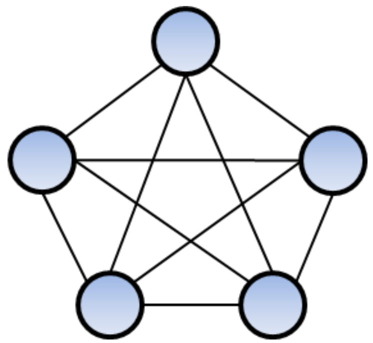
A graph where all possible edge connections between all nodes exist.

In a complete digraph, all the edges are bi-directional.

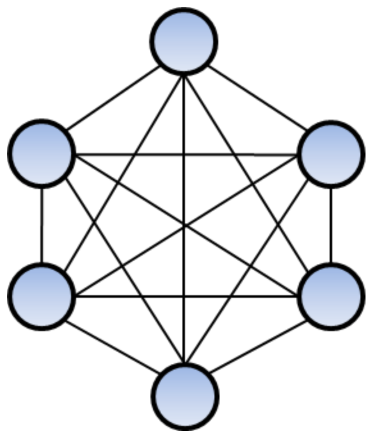
$$E = \binom{N}{2} = \frac{N(N-1)}{2}$$



4 nodes
6 edges



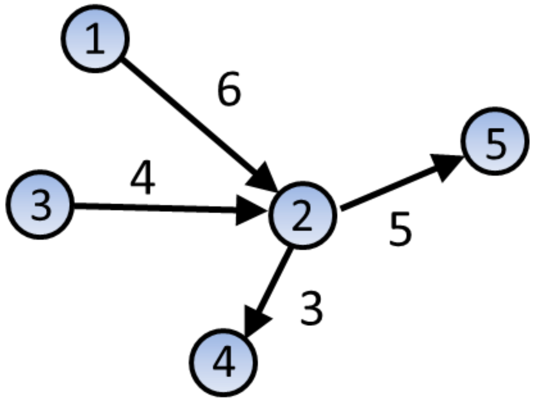
5 nodes
10 edges



6 nodes, 15 edges

Graph Representations

Different ways to represent graphs on code:



Source-Target-Weight Vectors

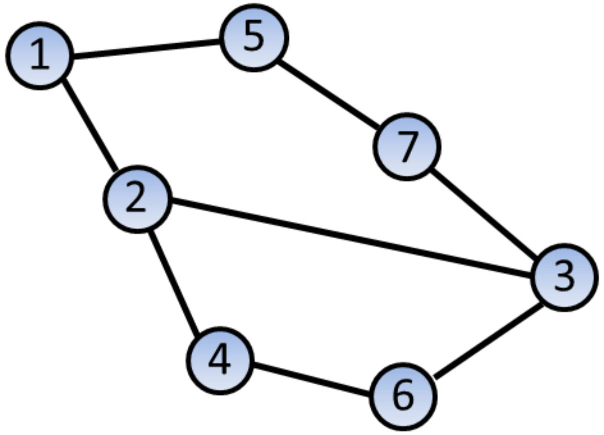
```
s = [1 3 2 2]
t = [2 2 4 5]
w = [6 4 3 5]
```

Adjacency Matrix

$$\begin{array}{cc} & \begin{array}{ccccc} N1 & N2 & N3 & N4 & N5 \end{array} \\ \begin{array}{c} N1 \\ N2 \\ N3 \\ N4 \\ N5 \end{array} & \begin{pmatrix} 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 5 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

Adjacency Lists

```
N1 [2]
N2 [4 5]
N3 [2]
N4 []
N5 []
```




```
s = [1 1 2 2 3 3 4 5]
t = [2 5 3 4 6 7 6 7]
```

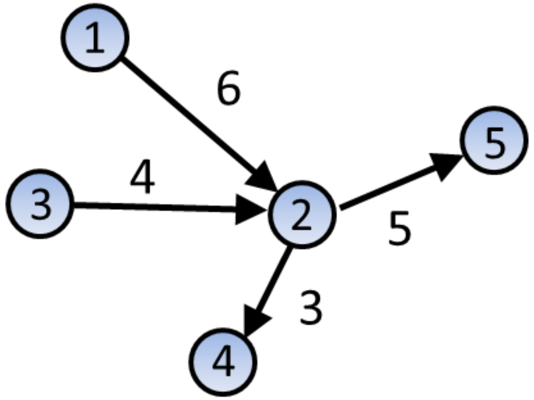
$$\begin{array}{cc} & \begin{array}{ccccccc} N1 & N2 & N3 & N4 & N5 & N6 & N7 \end{array} \\ \begin{array}{c} N1 \\ N2 \\ N3 \\ N4 \\ N5 \\ N6 \\ N7 \end{array} & \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

```
N1 [2 5]
N2 [1 3 4]
N3 [2 7 6]
N4 [2 6]
N5 [1 7]
N6 [3 4]
N7 [3 5]
```

Graph Terminologies

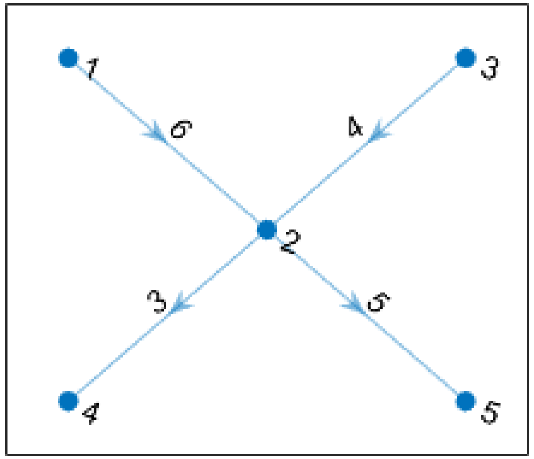
We can build graphs in MATLAB.

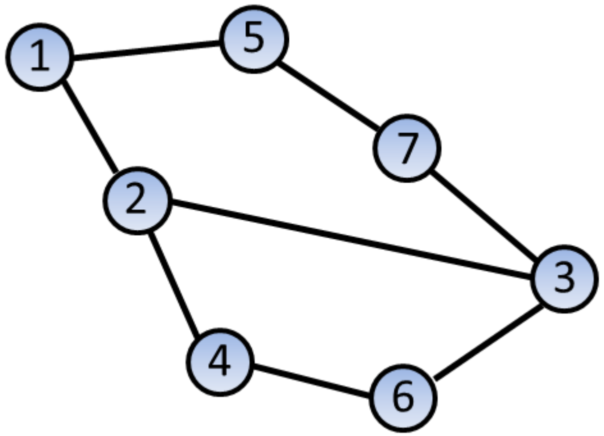
Enter the following codes:




```
>> s = [1 3 2 2];
>> t = [2 2 4 5];
>> w = [6 4 3 5];
>> G = digraph(s,t,w);
>> plot(G,'EdgeLabel',G.Edges.Weight);
```

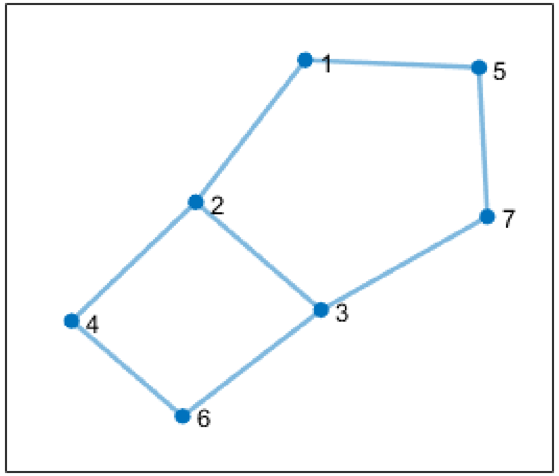
MATLAB output:
(verify that this graph is the same as the one on the left)






```
>> s = [1 1 2 2 3 3 4 5];
>> t = [2 5 3 4 6 7 6 7];
>> G = graph(s,t); plot(G);
```

MATLAB output:
(verify that this graph is the same as the one on the left)



Graph Algorithms

I. Reachability (Transitive Closure)
II. Topological Sorting
III. Shortest Path
IV. Max Flow
V. Minimum Spanning Tree

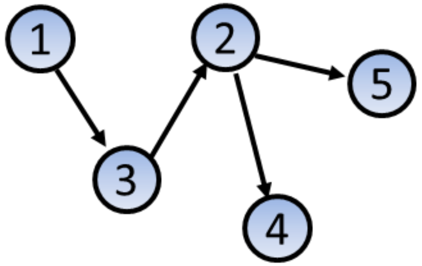
Reachability

Reachability: Is Node ‘T’ reachable from Node ‘S’?

Definition: Transitive closure.

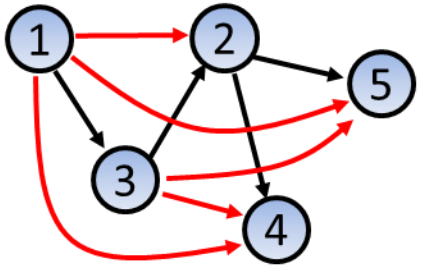
The *transitive closure* of a digraph *G* is another digraph with the same set of nodes, but where an edge from any S to T exists *if and only if* T is *reachable* from S in *G*.

Original Graph, G



$$\begin{bmatrix} 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & \mathbf{1} & \mathbf{1} \\ 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Transitive Closure of G



$$\begin{bmatrix} 0 & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} \\ 0 & 0 & 0 & \mathbf{1} & \mathbf{1} \\ 0 & \mathbf{1} & 0 & \mathbf{1} & \mathbf{1} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Related ChemE problems:

1. In a water distribution network, if a pumping station is down, which households are affected?
2. In a chemical plant, if a certain pipe is blocked, how will its effects propagate throughout the plant?
3. If a lake has been contaminated, which other sites in nature are affected?

Solution:

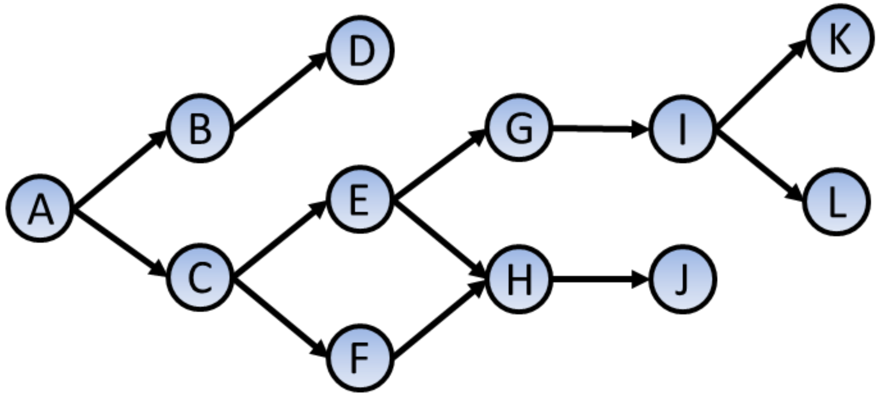
```
>> s = [1 2 2 3];
>> t = [3 4 5 2];
>> G = digraph(s,t);
>> H = transclosure(G);
>> full(adjacency(H))
```

In this new adjacency matrix, an entry of ‘**1**’ in *row S, column T* means that Node *T* is reachable from Node *S*.

Reachability

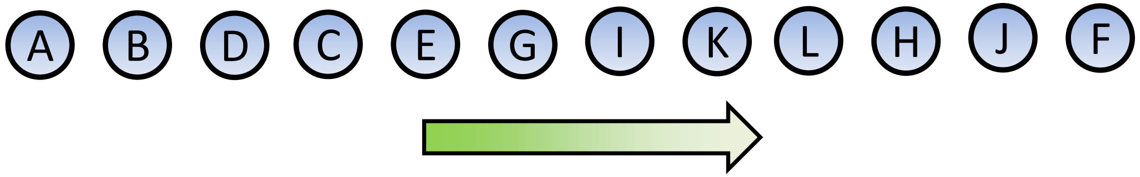
How can we traverse the entire graph from any starting Node *S*?

```
>> s = [1 1 2 3 3 5 5 6 7 8 9 9];
>> t = [2 3 4 5 6 7 8 8 9 10 11 12];
>> names = {'A','B','C','D','E','F',...
           'G','H','I','J','K','L'};
>> G = digraph(s,t,[],names)
```



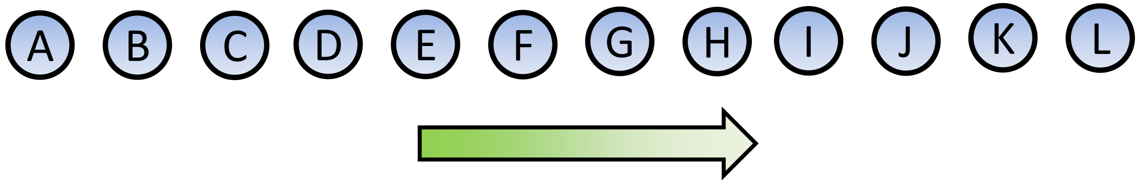
- **Depth-first search (DFS)**
  Go deep, move out, go deep again.
  ```
  >> visit = dfsearch(G,'A')'
  ```

Order of nodes visited by **DFS** starting from Node A.



- **Breadth-first search (BFS)**
  View all options, go to next level, view all again.
  ```
  >> visit = bfsearch(G,'A')'
  ```

Order of nodes visited by **BFS** starting from Node A.

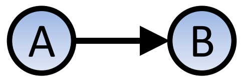


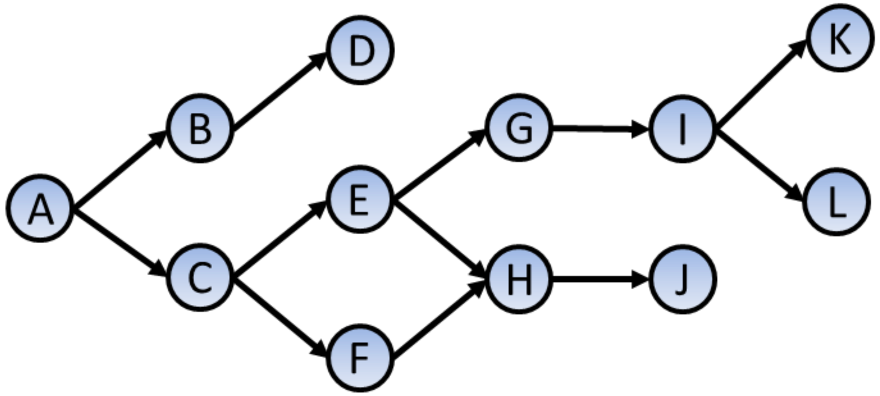
Topological Sorting

Given a graph of dependencies, how do we sort the nodes from left to right without violating their dependencies?

Example:

If an edge denotes *dependency*, then A must be performed before B.






```
>> s = [1 1 2 3 3 5 5 6 7 8 9 9];
>> t = [2 3 4 5 6 7 8 8 9 10 11 12];
>> names = {'A','B','C','D','E','F',...
           'G','H','I','J','K','L'};
>> G = digraph(s,t,[],names)
```

Related ChemE problems:

1. Given a set of tasks, where some must be performed before others, in which order should we perform them to minimize completion time?
2. In a batch process plant, how do we schedule the operation to complete all product orders in the shortest time possible?
3. Given a curriculum checklist for BS ChemE, find a possible ordering of subjects to be taken such that all pre-requisites are followed.

Solution:

```
>> N = toposort(G);
>> cell2mat(G.Nodes.Name(N,:)')

'ACFEHJGILKBD'
```

```
>> N = toposort(G,'Order','stable');
>> cell2mat(G.Nodes.Name(N,:)')

'ABCDEFGHIJKL'
```

If "stable", smaller node labels go first.

Note: `Toposort` does not require you to supply a starting node, whereas `dfsearch` does.

Graph Algorithms

I. Reachability (Transitive Closure)
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Shortest Path

Which path from Node S to T has the minimum sum of weights?

Example:

```
>> s = [1 1 1 2 2 2 3 3 4 5 6 7 7 8 8 9 9];
>> t = [3 5 8 4 5 9 2 9 7 3 4 1 6 4 7 6 7];
>> w = [7 20 13 12 7 6 4 8 3 5 5 6 5 7 12 10 10];
>> G = digraph(s,t,w);
>> p = plot(G,'EdgeLabel',G.Edges.Weight);
```

To find the shortest path from Node 1 to Node 6:

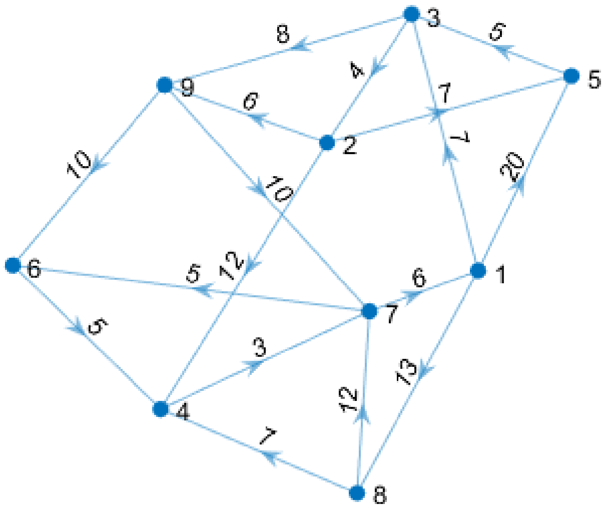
```
>> [path,d] = shortestpath(G,1,6);
>> highlight(p,path,'EdgeColor','g');
>> fprintf('Path length: %d\n',d);
```

Algorithms inside MATLAB's `shortestpath`:

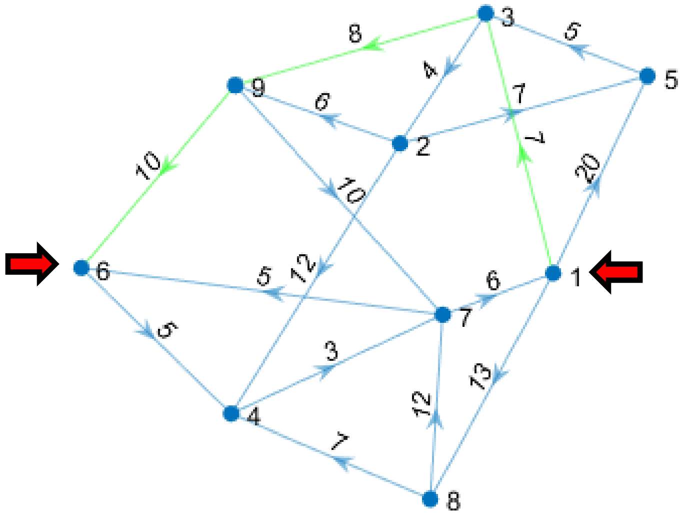
1. BFS (for unweighted)
2. Dijkstra (for digraph with all weights positive)
3. Bellman-Ford (for digraph with negative weights)

Related ChemE problems:

1. What is the fastest route to move goods geographically from source to demand?
2. Which path of reaction steps should be taken so that the net energy needed to create a target compound is minimum?
3. Which value chain would give a maximum net profit from a given raw material?



Answer: `Path length: 25`

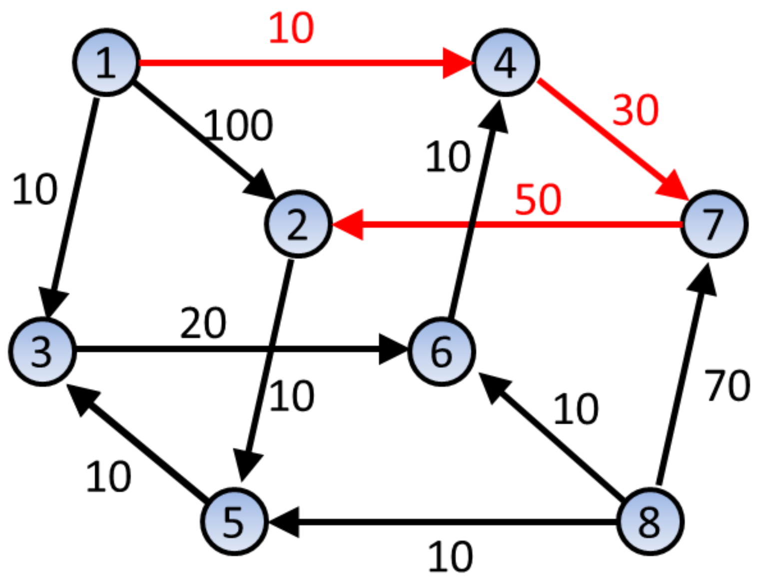


Shortest Path

Which path from Node S to T has the minimum sum of weights?

Example:

```
>> s = [1 1 1 2 5 3 6 4 7 8 8 8];
>> t = [2 3 4 5 3 6 4 7 2 6 7 5];
>> w = [100 10 10 10 10 20 10 30 50 10 70 10];
>> G = digraph(s,t,w);
>> plot(G,'EdgeLabel',G.Edges.Weight)
```



To find the shortest path between **any pair of nodes**:

```
>> D = distances(G);
```

D(i, j) is the length of the shortest path from node i to node j.

d = *8x8*

0	$\boxed{90}$	10	10	100	30	40	Inf
Inf	0	20	50	10	40	80	Inf
Inf	110	0	30	120	20	60	Inf
Inf	80	100	0	90	120	30	Inf
Inf	120	10	40	0	30	70	Inf
Inf	90	110	10	100	0	40	Inf
Inf	50	70	100	60	90	0	Inf
Inf	100	20	20	10	10	50	0

Graph Algorithms

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Max Flow

Given a *source* node S, a *sink* node T, and the flow capacity in each edge, find the maximum flow that can be pushed from S to T.

Related ChemE problems:

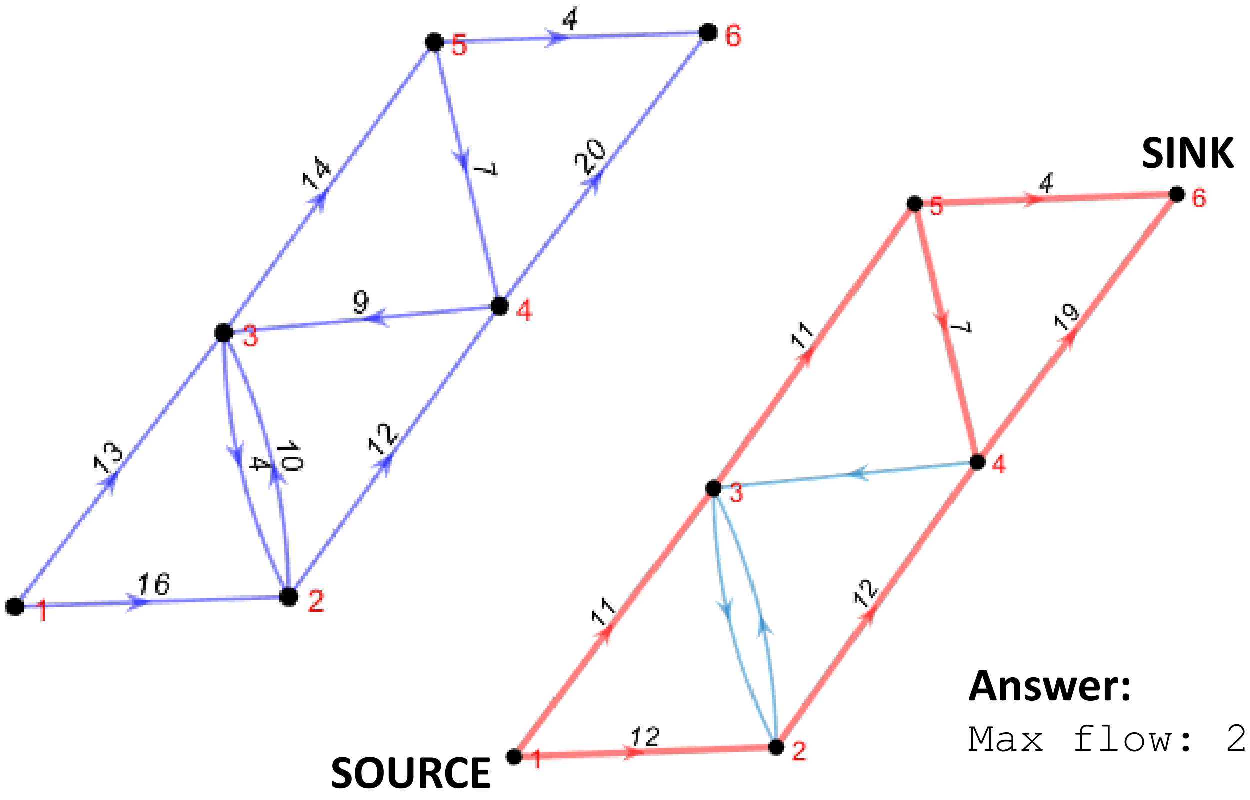
1. Find the maximum production capacity of a plant, given the capacity of each pipe and equipment.
2. Find the maximum no. of goods that can flow from the supply to the demand side, given that only a limited amount of goods can flow on certain roads.

Example:

```
>> s = 1; t = 6;
>> cap = [ 0 16 13 0 0 0;  0 0 10 12 0 0;
           0 4 0 0 14 0;   0 0 9 0 0 20;
           0 0 0 7 0 4;    0 0 0 0 0 0];
>> G = digraph(cap);
>> H = plot(G,'EdgeLabel',G.Edges.Weight)
```

To find the maximum flow (`mf`) from S to T and the resulting flow graph (`GF`):

```
>> [mf,GF] = maxflow(G,s,t);
>> H.EdgeLabel = {};
>> highlight(H,GF,'EdgeColor','r','LineWidth',2);
>> st = GF.Edges.EndNodes;
>> labeledge(H,st(:,1),st(:,2),GF.Edges.Weight);
>> fprintf('Max flow: %d\n',mf);
```



Answer:
`Max flow: 23`

Graph Algorithms

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Minimum Spanning Tree

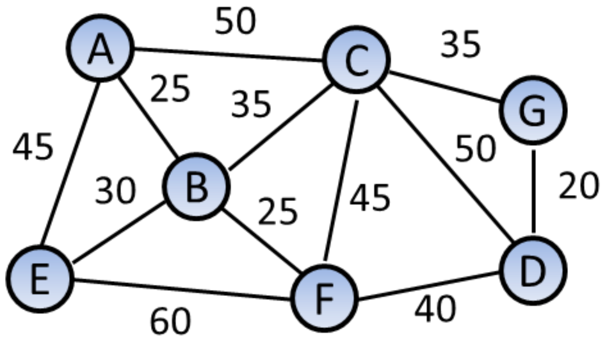
Given an undirected graph, find a subset of the edges such that the remaining graph is still connected but the total edge weight is minimum.

Example:

```
>> adj = [0 25 50 0 45 0 0;25 0 35 0 30 25 0;
          50 35 0 50 0 45 35; 0 0 50 0 0 40 20;
          45 30 0 0 0 60 0; 0 25 45 40 60 0 0;
          0 0 35 20 0 0 0];
>> G = graph(adj);
>> H = plot(G,'EdgeLabel',G.Edges.Weight)
```

To find the minimum spanning tree, T:

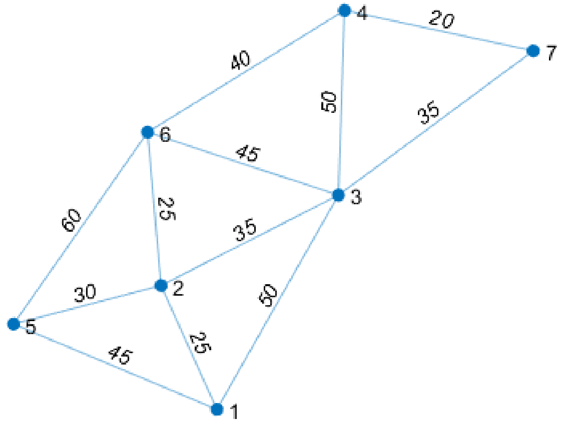
```
>> T = minspantree(G);
>> highlight(H,T);
```



Related ChemE problems:

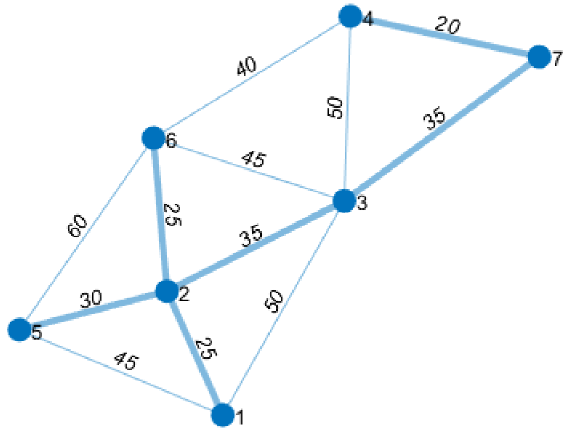
1. Given the geographical locations of power stations and loads, connect the entire power grid with the minimum total length of transmission cables.
2. Select only a few water lines to maintain during a water shortage, while ensuring that all households still have access to water.

MATLAB output:



Minimum spanning tree:

`Total weight: 170`



Summary

- There are optimization problems in ChemE that can be represented as graphs. Hence, graph algorithms are needed to solve them.

- You now have learned how to use new MATLAB built-in functions such as:

`graph`	`toposort`	`highlight`
`digraph`	`transclosure`	`adjacency`
`dfsearch`	`shortestpath`	`maxflow`
`bfsearch`	`distances`	`minspantree`