Graphs and network matrices

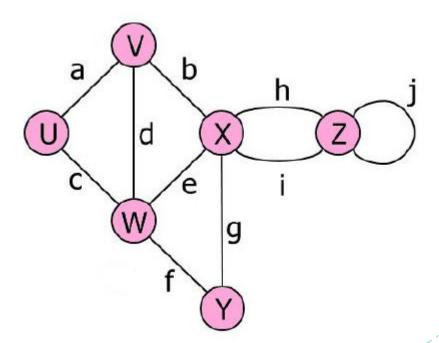
Olli-Pekka Hämäläinen

Graphs

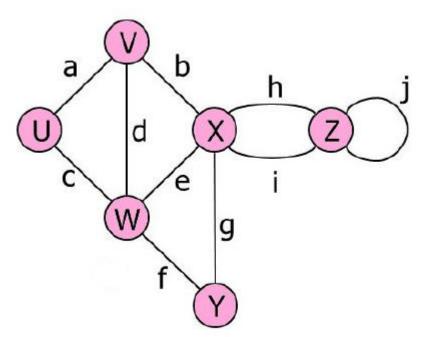
- We already used graphs in order to illustrate relations:
 - Domain-range-graph
 - Digraph (directed graph)
- Let's now get ourselves acquainted with graphs on general level in order to familiarize ourselves with terminology and gain more analysis tools
- With relations, the nodes of the graph were domain/range elements
 - Generally, in graphs these nodes are called vertices*
- Arrows represented the connections between domain/range elements
 - Generally, these are called edges
 - Can be either directed (as in arrows) or undirected
- This branch of mathematics that focuses on analysis of graphs is graph theory or network theory

*Personally I prefer the term "node" and will use that in these lectures.

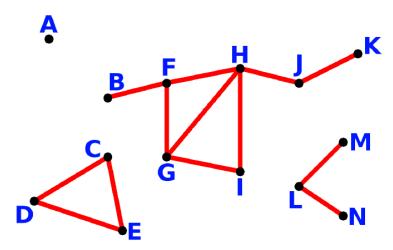
- Endpoints of an edge = nodes where the edge starts and ends (logically); for example, edge h has endpoints X and Z
- Edges a, b and d are connected to node V
- The *degree* of a node is the number of edges that are connected to it (example: degree of V = 3 & degree of W = 4



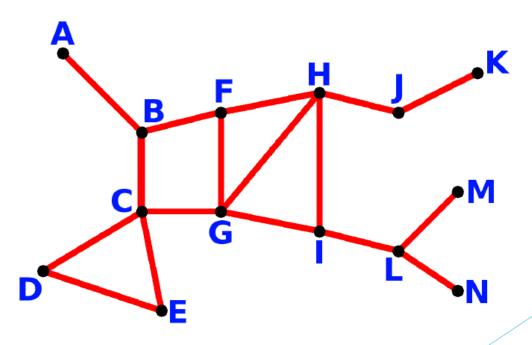
- Edges which have same endpoints are called parallel (for example, h and i here)
- If there is an edge between two nodes, these nodes are said to be *adjacent* (example: W and Y adjacent, Y and V are not)
- If the edge has only one endpoint, it's called a loop (example: j)



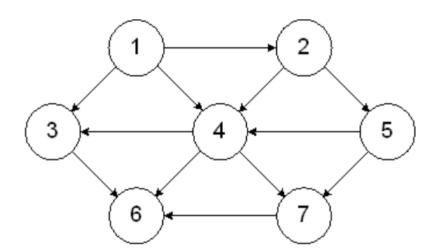
- If we can get from node X to node Y via one or several edges, there is a connection between X and Y a path
 - ► There can be several possible paths for example, here from B to I there are four: BFGI, BFHI, BFHGI, BFGHI
- If there exists a path between any two nodes, the graph is said to be *connected*
 - ▶ The graph below is not
- Nodes of degree 0 are called isolated nodes
 - In the graph below, A is an isolated node



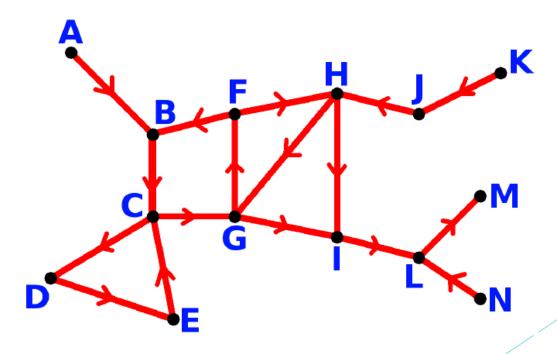
- If there is even one path that starts from arbitrary node X and comes back to it without travelling via the same edge twice, the graph is called *cyclic*
 - In the graph below, for example path BCGFB



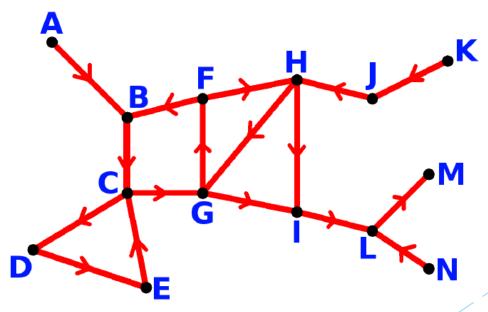
- In previous examples, the graphs were undirected so, the connections between nodes were automatically 2-way
- We can declare our edges to have a direction by marking the edge as an arrow
- This kind of graph is called a directed graph or digraph
 - We already used these to illustrate relations!



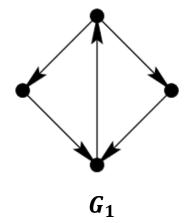
- The definition of a path is not changed in the case of digraph, but the number of possible paths is decreased
 - Example: now we can only get from B to I via path BCGI or BCGFHI
 - Going from I to B is impossible

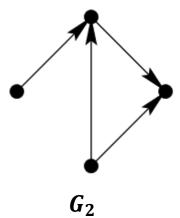


- The concept of degree of a node is split twice:
 - Indegree of a node = edges that arrive the node
 - Outdegree of a node = edges that leave the node
- If the indegree is zero, but the outdegree is not, the node is called a *source* (example below: A, K, N)
- If the outdegree is zero, but the indegree is not, the node is called a *sink* (example below: M)



- If the undirected graph that corresponds to the directed graph is connected, also the directed graph is connected
- If we can get from any node to any other node, the directed graph can be called *strongly connected* (graph G_1)
 - If the undirected graph is connected, but we can't get from any node to any other in the directed graph, the graph is called *weakly connected* (graph G_2)
- A strongly connected graph has no sources nor sinks





Choice of graph type

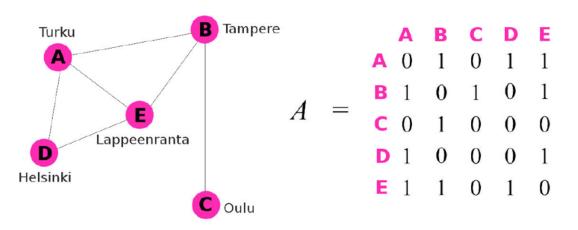
- Whether the graph should be directed or not, and what kind of structures the graph is allowed to have, depends naturally on the process or situation to be modeled
 - For example, road networks are usually undirected unless there are one-way streets in the network
- Undirected graphs are often "denied" the option to possess parallel edges or loops
 - If such structures exist, the graph is actually a *multigraph*
 - Most source books use the word "graph" quite vaguely as a general term - even though a graph is a special case of a multigraph
 - In order to make distinctions, graphs that have no parallel edges or loops, are often referred to as *simple graphs*

Network matrices

- Small graphs are easy to analyze graphically, but as the size of the graph increases, analysis gets tougher
 - Best option is to take advantage of computers
- The easiest way to define a graph for a computer is to describe it via network matrices
 - Notions "graph" and "network" have no fundamental difference
 - Some sources do link the notion "network" only to directed graphs, though
- Let's familiarize ourselves with some network matrices
 - Applications are mostly left for follow-up courses

Adjacency matrix A

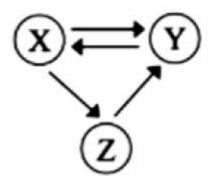
- Adjacency matrix describes which nodes are adjacent to each other (as the name suggests)
 - Nodes as rows and columns \rightarrow always a square matrix
 - If there is an edge* from node i to node j, the value of element a_{ii} of the adjacency matrix is 1 (otherwise 0)
 - Diagonal elements either 0 or 2 (if the node has a loop)
- The adjacency matrix of an undirected graph is always symmetric (example: train network between cities)



*Or, in case of multiple parallel edges, a_{ii} = number of edges

Adjacency matrix A

- In a directed graph, directions are taken into account:
 - ▶ If there is an arrow from node i to node j, then $a_{ii} = 1$
 - ► This arrow doesn't make element a_{ii} to one
- Therefore, the adjacency matrix of a directed matrix is not (usually) symmetric
- The relation matrices we used during the previous week are actually adjacency matrices of relation digraphs!

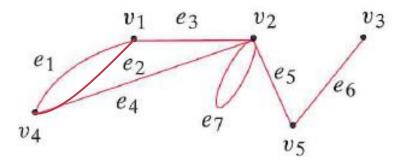


	X	Y	Z
X	0	1	1
Y	1	0	0
Z	0	1	0

- Another possible way to depict a graph in matrix form is to define its incidence matrix
 - Rows are nodes $(x_i \text{ or } v_i)$, columns are edges (e_i)

$$b_{ij} = \begin{cases} 1, & \text{if } e_j \text{ is connected to node } x_i \\ 0, & \text{otherwise} \end{cases}$$

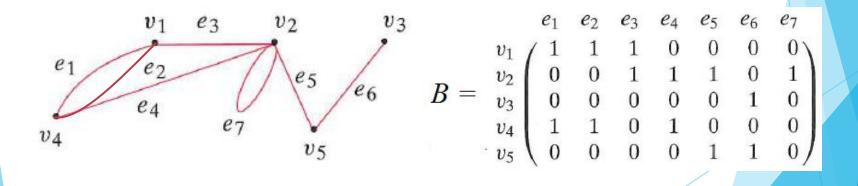
NOTE! This is not a square matrix (unless in special cases)



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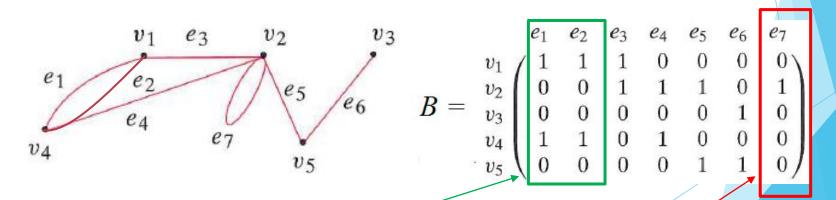
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Identical columns = edges 1 and 2 are parallel!

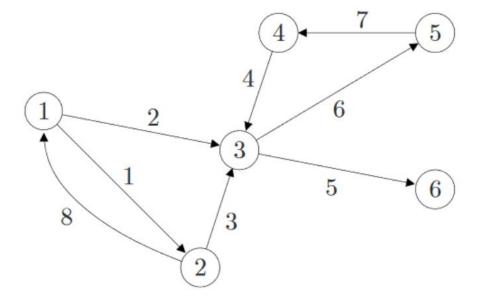
Columns that have just one 1 = loops

In case of a directed graph, the edges (= arrows) can get either a positive or negative value - depending on the direction of the arrow:

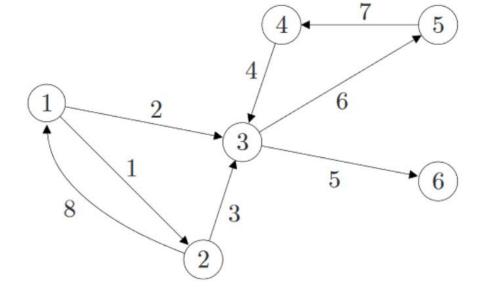
$$b_{ij} = \begin{cases} 1, & \textit{if arrow j starts from node i} \\ -1, & \textit{if arrow j ends in node i} \\ 0, & \textit{otherwise} \end{cases}$$

- Incidence matrix is usually greater in size than adjacency matrix (depends on the number of edges, though)
- Removal of careless errors: because each column corresponds to one edge, each column must have at most two 1s (undirected graph) or 1 and -1 (directed graph)

Example:



Example:

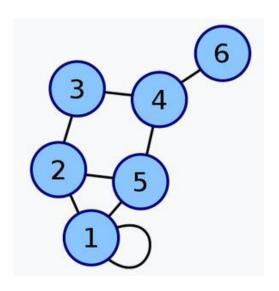


$$B = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & -1 & -1 & -1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \end{bmatrix}$$
Nodes as rows (6 pcs)

Arrows as columns (8 pcs)

Degree matrix D

- Degree matrix specifies, how many edges are connected to each node - so, degrees of nodes
 - Nodes as rows and columns → always a square matrix
 - Pure diagonal matrix
 - ► Loops are calculated twice (because a loop both starts and ends in same node); this is why here degree of node 1 = 4



$$D = \begin{pmatrix} 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Degree matrix D

- In case of a directed graph, the degree matrix has three alternative interpretations:
 - Degree matrix of the corresponding undirected graph
 - Indegree matrix of the directed graph
 - Outdegree matrix of the directed graph
- Pay attention to definitions when reading sources!
- Usually, if text just says "degree matrix" with a directed graph, this means the first alternative
 - If the degree matrix is linked to indegrees or outdegrees, this is specifically mentioned

Laplace matrix L

- In deeper graph analysis, one commonly needed tool is Laplace matrix
- This can be defined via previously introduced matrices
 - 2 possible methods
- Directed graph: product of incidence matrix and its transpose

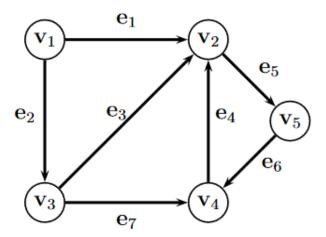
 $L = BB^T$

- NOTE: for undirected graphs, $L = BB^T 2A$
- Undirected graph: Difference of degree matrix and adjacency matrix

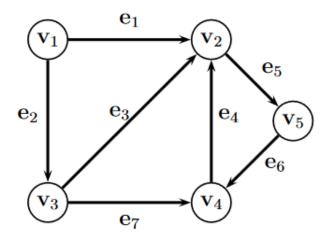
$$L = D - A$$

NOTE: This can be used for directed graphs, too - in this case, D and A must be the degree and adjacency matrices of the corresponding undirected graph

▶ Directed graph G_1 is as follows:



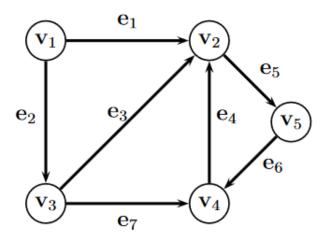
Directed graph G₁ is as follows:



Incidence matrix

$$B = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 \end{pmatrix}$$

Directed graph G_1 is as follows:



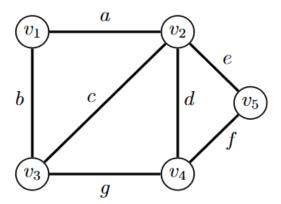
Incidence matrix

$$B = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 \end{pmatrix} \quad A(G_1) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

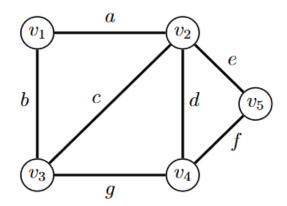
and adjacency matrix

$$A(G_1) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

 \triangleright Convert the graph to an undirected graph G_2 :



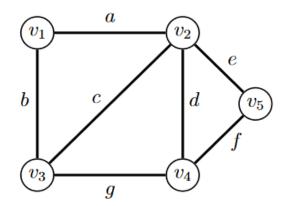
Convert the graph to an undirected graph G₂:



Adjacency matrix of G₂

$$A(G_2) = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix}$$

 \triangleright Convert the graph to an undirected graph G_2 :



Adjacency matrix of G₂

and its degree matrix

$$A(G_2) = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{pmatrix} \quad D = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

Laplace matrix using incidence matrix: directed graph, so

$$L = BB^{T} = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 4 & -1 & -1 & -1 \\ -1 & -1 & 3 & -1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{bmatrix}$$

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 \triangleright ...or, by using degree and adjacency matrices of G_2 :

$$L = D - A(G_2) = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix} - \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

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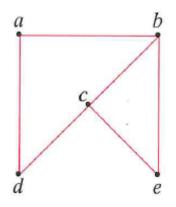
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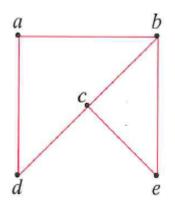
- Which matrix (A or B) should we use, then?
 - If there are more edges than nodes in the graph (most common situation), adjacency matrix is smaller and requires less space & calculation time; therefore, it is also more commonly used
 - If there are less edges than nodes, incidence matrix is smaller
 - ▶ One bonus of B: enables separation of parallel edges!
- Degree numbers of nodes can be seen directly from the adjacency matrix by calculating row and column sums
- In an incidence matrix, degrees of nodes can be calculated from row sums
 - Column sums are always either 0 (directed graph), 1 (loop) or 2 (undirected graph)

- For a simple undirected graph, the powers of adjacency matrix have a special meaning:
 - Element a_{ij} of matrix Aⁿ tells the number of different possible n-step paths from node i to node j
 - In other words: in how many ways can we travel from node i to node j via n pcs of edges



$$A = \begin{pmatrix} a & b & c & d & e \\ a & b & 1 & 0 & 1 & 0 \\ b & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ e & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

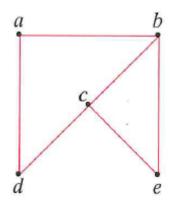
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$$A = \begin{pmatrix} a & b & c & d & e \\ a & b & c & d & e \\ b & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ e & 0 & 1 & 1 & 0 & 0 \end{pmatrix} \qquad A^2 = \begin{pmatrix} a & b & c & d & e \\ 2 & 0 & 2 & 0 & 1 \\ 0 & 3 & 1 & 2 & 1 \\ 2 & 1 & 3 & 0 & 1 \\ 0 & 2 & 0 & 2 & 1 \\ 1 & 1 & 1 & 1 & 2 \end{pmatrix}$$

$$A^{2} = \begin{pmatrix} a & b & c & a & c \\ b & 2 & 0 & 2 & 0 & 1 \\ 0 & 3 & 1 & 2 & 1 \\ 2 & 1 & 3 & 0 & 1 \\ 0 & 2 & 0 & 2 & 1 \\ e & 1 & 1 & 1 & 2 \end{pmatrix}$$

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Example: from node a to node c using 2 steps, there are 2 path options (abc, adc). From node c to node c using 2 steps, there are 3 path options (cbc, cdc, cec).

Properties of Laplace matrix

- Laplace matrix is always symmetric
- All row and column sums are zero
- All eigenvalues are positive
- Laplace matrix and its eigenvalues can be used for many purposes - for example:
 - Minimal spanning tree search
 - Other network optimization problems
 - Computer vision and machine learning solutions
- The actual applications are left for follow-up courses
 - Ask Jouni Sampo during matrix calculation course ©

Thank you!

