Analysis of Complex Systems

Lecture 2: Complex systems as graphs

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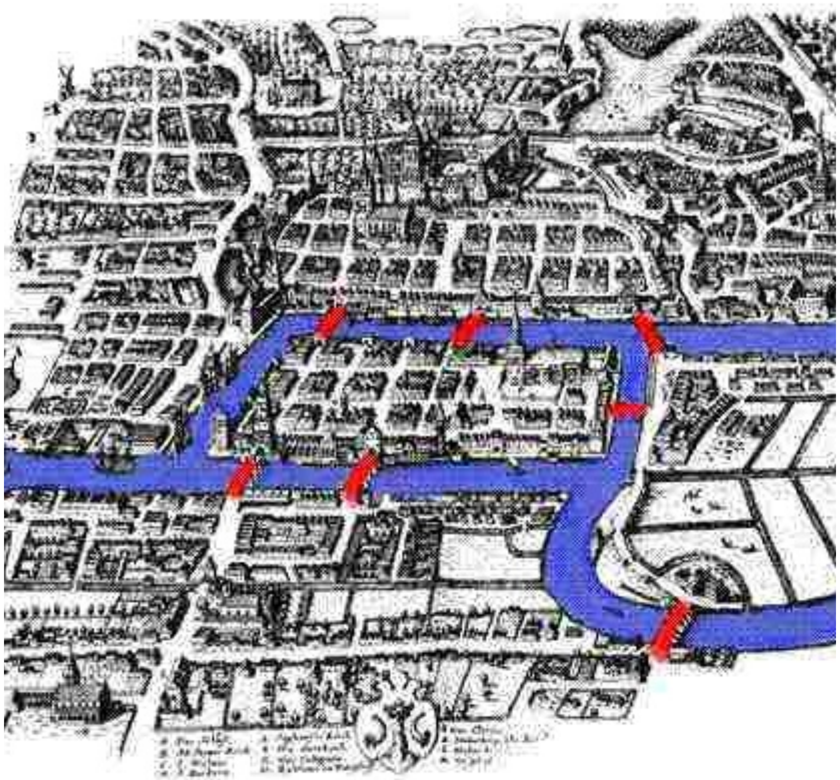
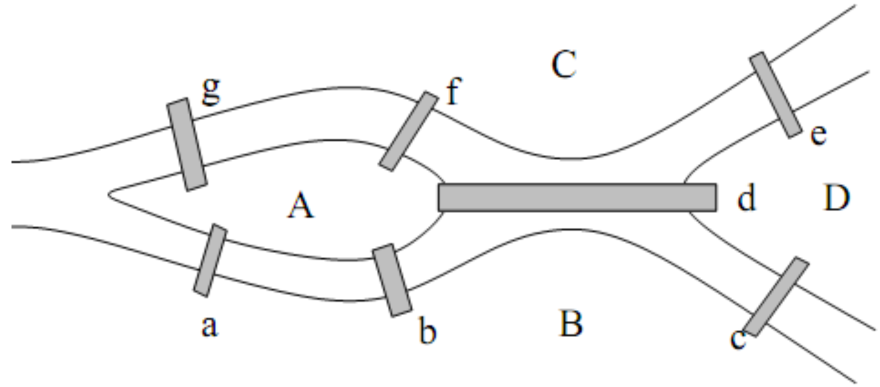
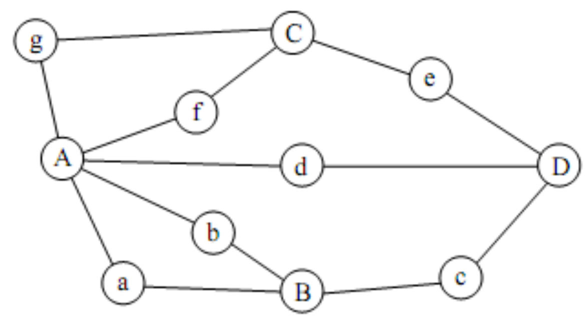
Objectives

- Graphs
- Computational complexity (Time and Space)
- Graph representations
- Patterns in graphs
- (Shortest) Paths

Origin of graph theory: Leonhard Euler, 1736







Bridges over the river Pregel in Königsberg (now Kaliningrad)
Euler tour: path that visits each edge and returns to the origin

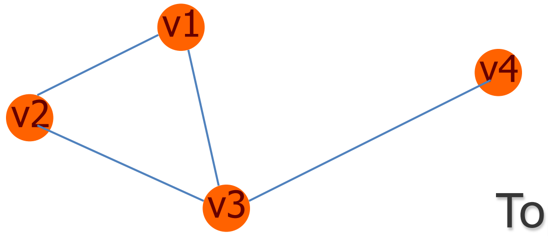
Graphs

- Graph: set of nodes and edges (non-directed)

  $$G = (V,E)$$

- Set of nodes: V (singular: vertex; plural: vertices)
- Set of edges: $E \subseteq V \times V$
- E.g., V={v1,v2,v3,v4},

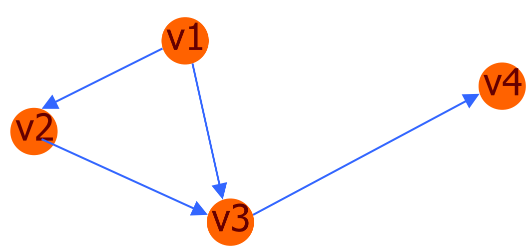
  E={(v1,v2), (v1,v3), (v2,v3), (v3,v4)}



Topology (rare term: hodology)

Directed graphs (Digraphs)

- Graph: set of nodes and *arcs* (directed)
- Set of nodes (vertices): V
- Set of edges: E $\subseteq$ V x V, the order matters
- E.g., V={v1,v2,v3,v4},
  E={(v1,v2), (v1,v3), (v2,v3), (v3,v4), (v4,v1)}



Graphs and Networks

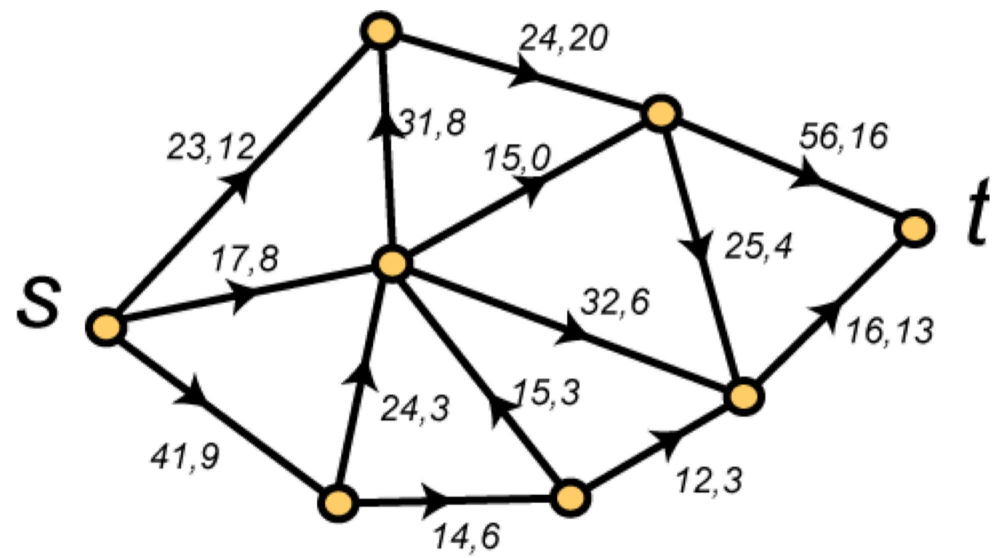
In theory (mathematics)

Graph: G=(V,E)

Network: N=(G, s, t, c)

defined by graph G with source s, sink t, and edge capacity c

(examples: electricity/power grid, water flow, metabolic flux)



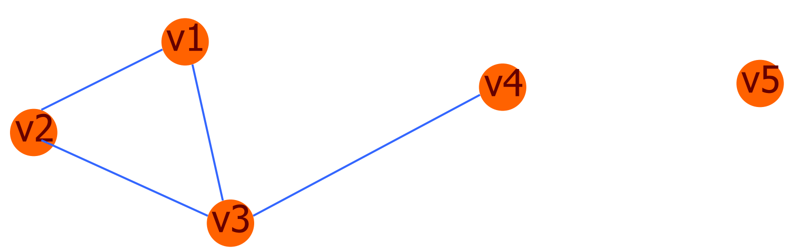
In reality (CS, engineering, economics, life and social sciences):

term network used throughout (as in this course)

Nodes in graphs

- Isolated nodes
- Degree of a node
- Connected graph
- Average degree of a graph
- Edge density: probability that any two nodes are connected
  $$d = \frac{E}{(N*(N-1))/2)}$$

- Isolated node: v5
- Degree of a node:
  d(v1)=2, d(v4)=1
- Average degree of a graph:
  D = (2+2+3+1+0)/5 = 1.6
- Edge density
  d=4/(5*4/2) = 0.4



Examples: edge density

	nodes	edges	density [%]
Autobahnen	1 168	2 486	0.18
Internet	6 524	29 629	0.0696
www	325 729	1 497 135	0.0014
Power Grid	4 677	12 500	0.0572
metabolic	422	1 972	1.3
C. Elegans	202	2 540	6.3
(partial network)			
macaque	73	835	16

sparse network
(density ~ 1%)

dense network
(density > 5%)

Algorithm evaluation: Time and space

Computational resources

- Two resources constrain our analysis and simulations: processing *time* and memory *space*
- How much time and space will an algorithm need to deal with a network with N nodes? Are there better algorithms that are faster or use less memory?

Big-O notation gives a *worst-case* approximation of needed resources. Examples:

Resource needed	Big-O notation
$c*N$	$O(N)$ (constant factors are neglected)
N^2+N+c	$O(N^2)$ (only largest component of a sum is used)

Examples for the time resource

(P – polynomial)

The good:

time to get an item from a table: $O(1)$

time needed for adding N numbers: $O(N)$

The bad:

calculate the degree of all nodes $O(N^2)$

find all shortest paths $O(N^3)$

(NP – non-polynomial)

N*(N-1)*(N-2)*…*3*2*1

The ugly:

test whether two networks are identical: $O(N!)$

travelling salesman problem: $O(N^N)$

Graph representation

Representation of graphs – 1

- Adjacency matrix: a(i,j) = 1 if there is an edge between nodes i and j, a(i,j)=0 otherwise
- In case of non-directed graphs the adjacency matrix is symmetric (same values across the diagonal)
- In case of directed graphs the adjacency matrix may not be symmetric

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

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

Advantage: Direct access to each element (O(1) time complexity)

Disadvantage: Storage needs for large networks (space complexity $O(N^2)$ even if most entries are zeros)

Representation of graphs – 2

- Adjacency list (list of existing edges)
- $E=\{(v1,v2,w_{12}),$
  $(v1,v3,w_{13}),$
  $(v2,v3,w_{23}),$
  $\ldots\}$

  w: weight (e.g. 1)

Can be generated in Matlab with the *sparse* command

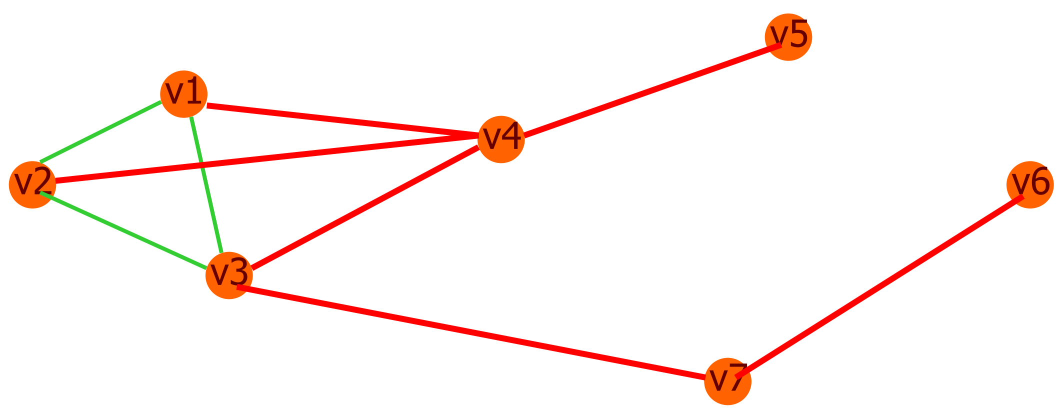
Advantage: Low demand for computer memory
(space complexity: O(E) ~ O(N))

Disadvantage: time to access one matrix element
(time complexity O(E) instead of O(1) for adjacency matrices:
worst case fully connected matrix $O(E) = O(N^2)$)

Patterns in graphs

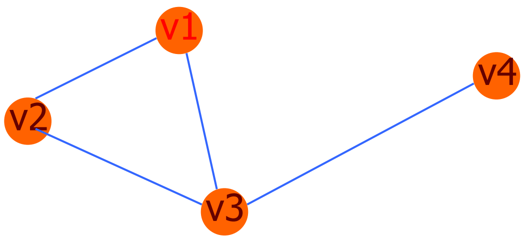
Sub-graphs

- Sub-graph = subset of edges and nodes
- E.g., $E' \subseteq E$, $V' \subseteq V$
- Complementary graph = the rest of the graph



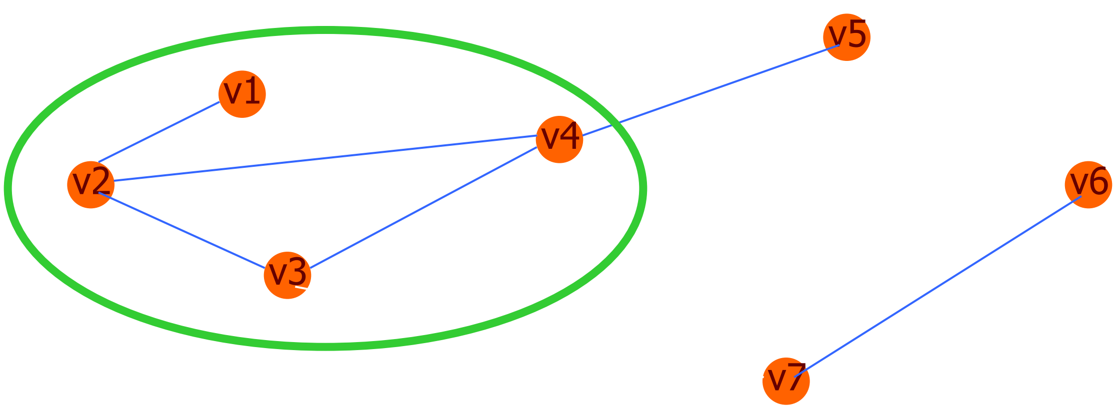
Neighbourhood

- Neighbourhood of a node = set of nodes connected to the node
- E.g., N(v1)={v2,v3}
- E.g., close functional relationship

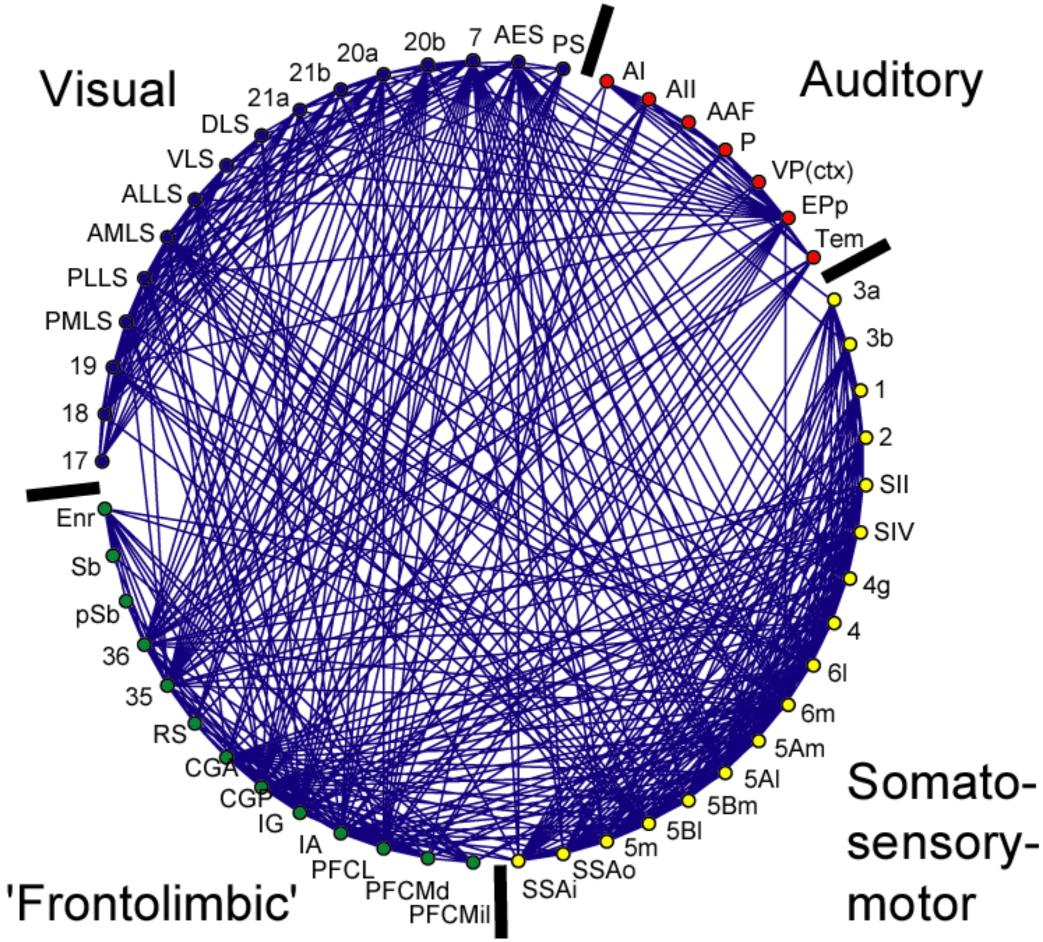


Clusters (or modules / communities)

- Dense connections within subgraph but few connections with remaining network
- Nodes within clusters often have similar functions (e.g. protein interaction cluster)



Example: Cat cortical connectivity



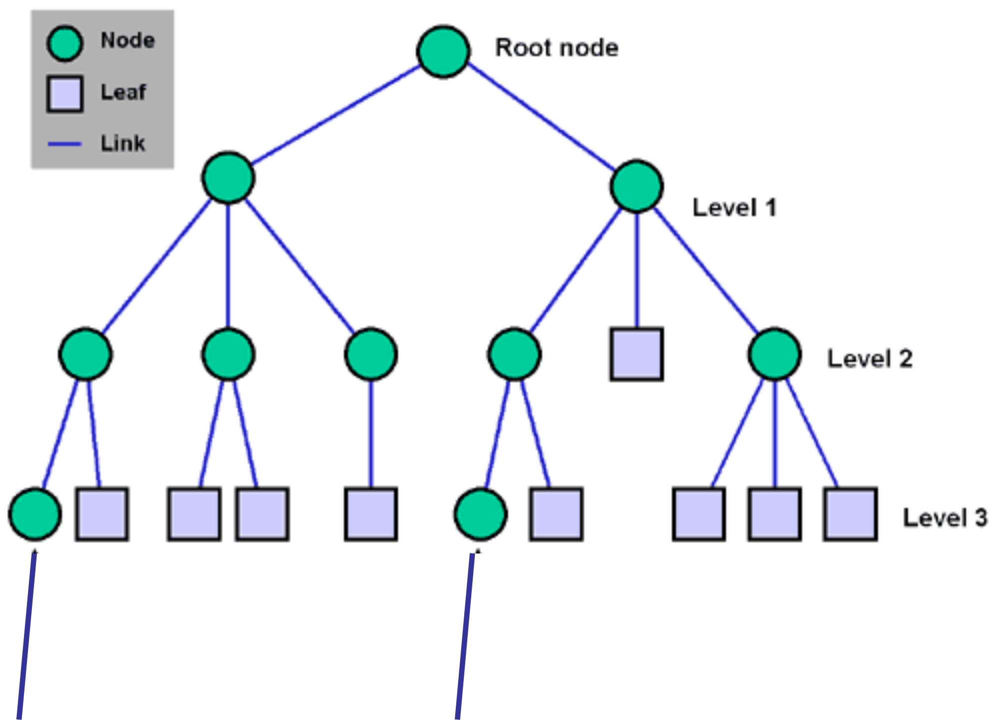
Edge: Existing fibre tract

Colours: Area function

Position: Nearby on the circle when connections are similar

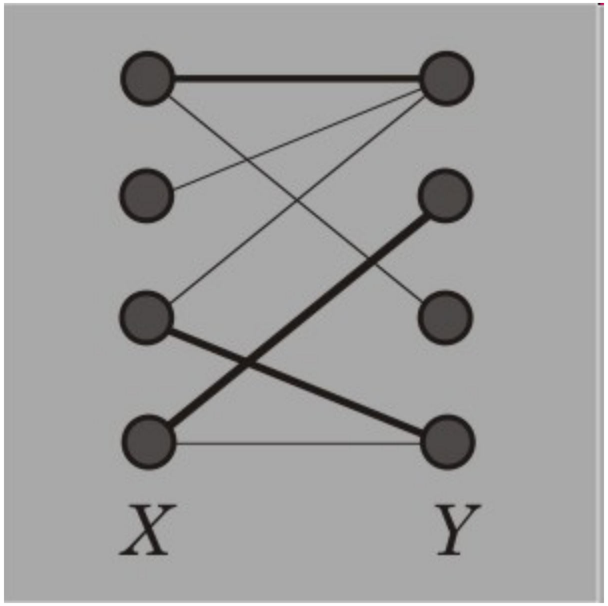
Trees

- Tree = set of nodes and edges, such that *no cycle* is included
- Terminology: forest, parent, leaf, root



Bi-partite graphs

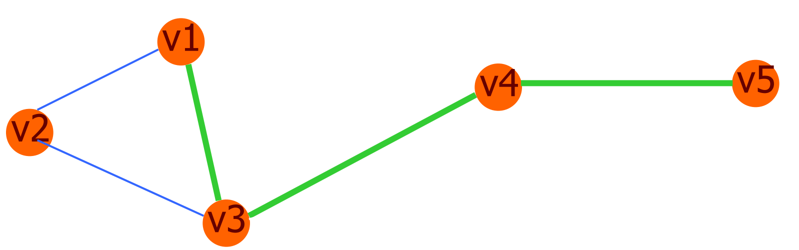
- Subclass of n-partite graphs
- Two classes:
  only edges between nodes of a different class are established
- Examples:
  Pairing (male-female; people-guitars)
  Interactions (DNA-Protein)



(Shortest) Paths

Paths in graphs – 1

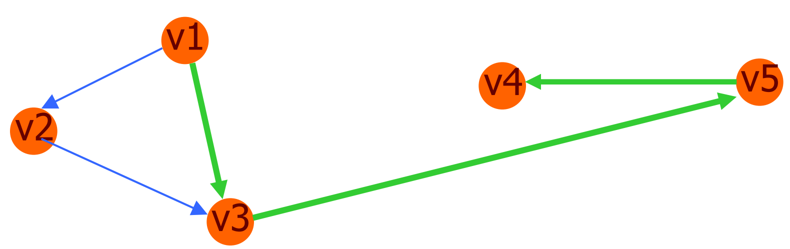
- Path between nodes
- E.g., signalling pathway
- E.g., V={v1,v2,v3,v4,v5,v6}, E={(v1,v2), (v1,v3), (v2,v3), (v3,v4), (v3,v5), (v5,v4)}
  P(v1,v5)={(v1,v3),(v3,v4),(v4,v5)}



Paths in graphs – 2

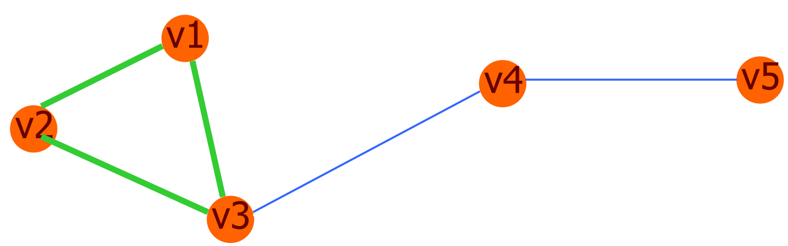
- Directed graphs
- E.g., V={v1,v2,v3,v4,v5,v6}, E={(v1,v2), (v1,v3), (v2,v3), (v3,v4), (v3,v5), (v5,v4)}

  P(v1,v5)={(v1,v3),(v3,v5),(v5,v4)}



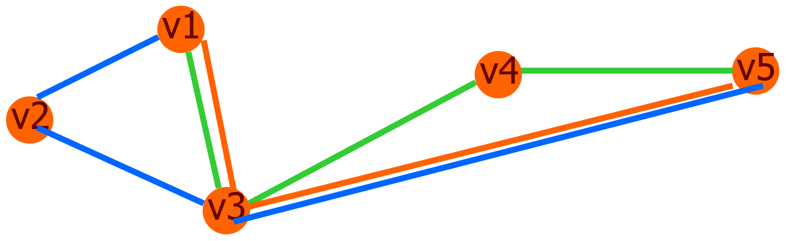
Paths in graphs – 3

- Cycles (non-directed) and circuits (directed)
- E.g., metabolic cycles
- E.g., C=(v1,v2,v3)
- Loop = direct feedback (v1->v1)



Paths in graphs – 4

- Number of paths between two nodes
- E.g., how redundant are protein interaction systems
- E.g., P(v1,v5)={(v1,v3),(v3,v5)}, {(v1,v3),(v3,v4),(v4,v5)}, {(v1,v2),(v2,v3),(v3,v5)}



Paths in graphs – 5

- Length of path: number of edges in the path
- E.g., P(v1,v5)={(v1,v3),(v3,v5)}, length (P)=2
- Paths of length 1 → entries of the adjacency matrix A
- Paths of length 2 → entries of $A^2 = A \times A$
- Paths of length k → entries of $A^k = A \times A^{k-1}$

Matrix multiplication

- Element-wise multiplication (A.*B = C in Matlab)

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

- Matrix multiplication (A*B = C in Matlab)

  A x B

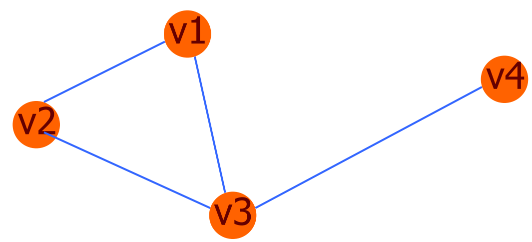
$$c_{i,j} = a_{i,1}b_{1,j} + a_{i,2}b_{2,j} + \dots + a_{i,n}b_{n,j}$$

$$C_{i,j} = \sum_{r=1}^{n} A_{i,r}B_{r,j}$$

Paths in graphs – 6

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

$$A^2 = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 3 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}$$

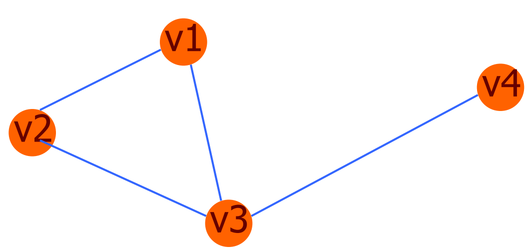


$$A^3 = \begin{pmatrix} 2 & 3 & 4 & 1 \\ 3 & 2 & 4 & 1 \\ 4 & 4 & 2 & 3 \\ 1 & 1 & 3 & 0 \end{pmatrix}$$

$$A^4 = \begin{pmatrix} 7 & 6 & 6 & 3 \\ 6 & 7 & 6 & 3 \\ 6 & 6 & 11 & 2 \\ 4 & 4 & 2 & 3 \end{pmatrix}$$

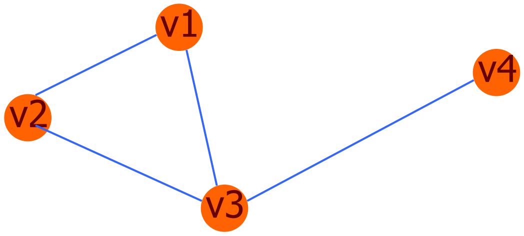
Paths in graphs – 7

- Distance between two nodes = length of minimal length path between the nodes
- D(v1,v4) = min {
  length({(v1,v3),(v3,v4)}),
  length({(v1,v2),(v2,v3),(v3,v4)})
  } = 2



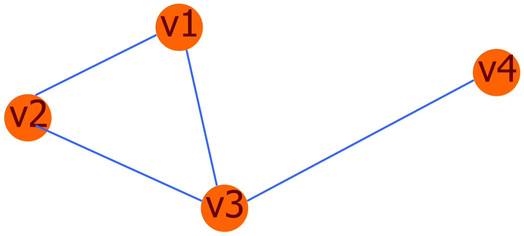
Paths and graphs – 8

- Diameter of a graph = maximum of distances between nodes of the graph
- D(G) = max {d(v1,v2), d(v1,v3), …, d(v3,v4)} = 2



Paths and graphs – 9

- Average distance of a graph
  (or average shortest path / *characteristic path length*)
  = average of distances between nodes
- Example:
  D(G) = (d(v1,v2) + d(v1,v3) + … + d(v3,v4)) / 12



Time complexity: $O(N^3)$; some algorithms achieve $O(N^2 \log N)$

Examples: average path length

- Human acquaintance network: 7 steps ("six degrees of separation") between any two persons in the US (Milgram, Psychology Today, 1963) -> small-world phenomenon

- World-Wide-Web: 19 steps from one web page to any other webpage (Albert et al., Nature, 1999)

- Neural networks:
  C. elegans: 2 steps (Watts & Strogatz, Nature, 1998)
  Macaque and cat fibre tract networks: 2 steps (Hilgetag, Phil. Trans. Roy. Soc. B, 2000)

Summary

- What are graphs and patterns in graphs?
- Which time and space resources are needed to analyse this size of the network? Are there better algorithms?
- How can networks be represented in the computer and what are the benefits and disadvantages?
- What are paths/shortest paths/diameter?

Q&A – 1

1. Is it true that graphs are made of nodes and edges ?
2. Is it true that in a directed graph the edge (v1,v2) is equivalent with the edge (v2,v1) ?
3. Is it true that it is possible to have more than one path between two nodes of a graph ?
4. Is it true that the distance between two nodes is the length of the longest path between the two nodes ?

Q&A – 2

5. Is it true that the matrix A is an adjacency matrix ? What about the matrix B ?

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

Q&A – 3

6. Is it true that the neighbourhood of a node is the set of nodes connected to the node ?
7. What is the time and space complexity of the following tasks:
   - yield all neighbours of one node
   - yield the length of the longest path between one pair of nodes
   - yield the all alternative shortest paths between one pair of nodes