



Lecture 3 - The algebra of networks' graphs

Graph-Based Data Science For Networked Systems
ECE 5260 – ORIE 5735

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1 Walk, Trail, Path, Cycle

- Distance between nodes

2 Algebra of networks

- Premise
- Adjacency matrix

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Outline



1 Walk, Trail, Path, Cycle

2 Algebra of networks

3 Conclusion



Moving on a graph

- In some applications the data of interest can be modeled as the *sequence of nodes visited on a graph*
- These visits of nodes in many cases are modeled as a stochastic process called **random walk**
- Irrespective of the domain application how easy it is to navigate the entire graph is often a feature of interest to understand how efficient is the interaction in the network, since it affects
 - how graph nodal data can change in light of a triggering event that propagates through the network
 - how well goods, money, data, opinions, viruses flow and spread in an network.



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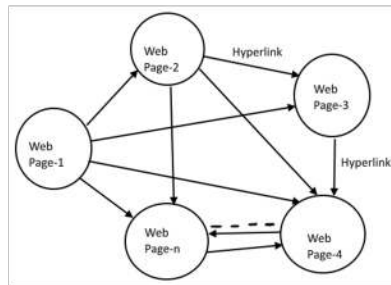
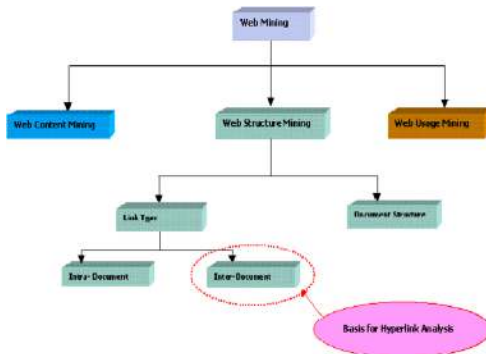


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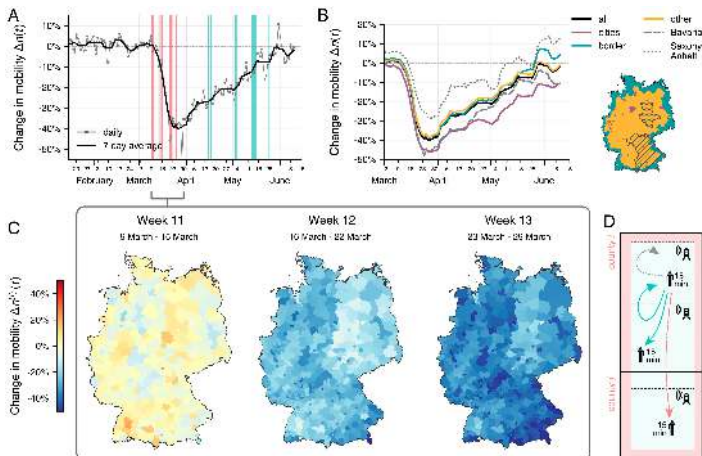
Example: browsing trends

- For example, in webometrics the classic example is the users browsing history is the pattern in which users navigate hyperlinks (a *fingerprint* for the user)



Example: epidemics

- This is an example where the dynamics of the spread of a state (virus infection, idea, failure) are affected by navigating the human network





Moving on a graph: walk

Graphs topological characteristics

Walk

A walk is a sequence alternating vertexes and the edges that connect them and ending with a node.

$$\mathfrak{w}_{v_0, v_n} = \{v_0, e_1, v_1, \dots, v_{n-1}, e_n, v_n\}.$$

The length of the walk is n , i.e. the number of edges in $\mathfrak{w}$.

Open walk

A walk is said to be an open walk if the starting and ending vertices are different i.e. the origin vertex and terminal vertex are different.

Closed walk

A walk is said to be a closed walk if the starting and ending vertices are identical.



Moving on a graph: walk

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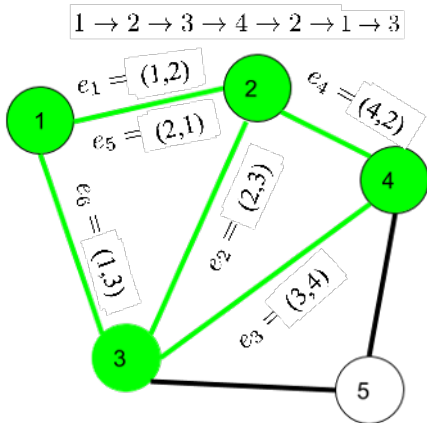
Closed walk

A walk is said to be a closed walk if the starting and ending vertices are identical.



Example of walk

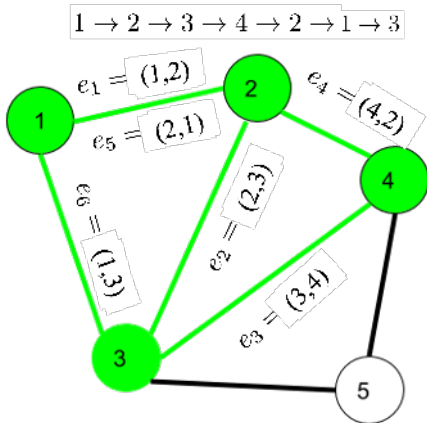
- The nodes are visited multiple times in general.
- $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 2 \rightarrow 1 \rightarrow 3$ (shown in the figure) is a walk (more specifically an open walk)
- The first five steps of the walk are $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 2 \rightarrow 1$, which is a closed walk.





Example of walk

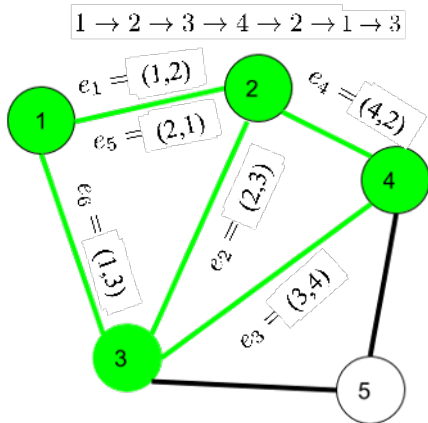
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Trail and circuit

Graphs topological characteristics

Trail

A **trail** between two nodes $t_{u,v}$ is a walk without repeated edges.

Circuit

A **trail** is a closed trail. Can have repeated vertices only. Note that nodes can be visited multiple times in a trail.



Trail and circuit

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Graphs topological characteristics

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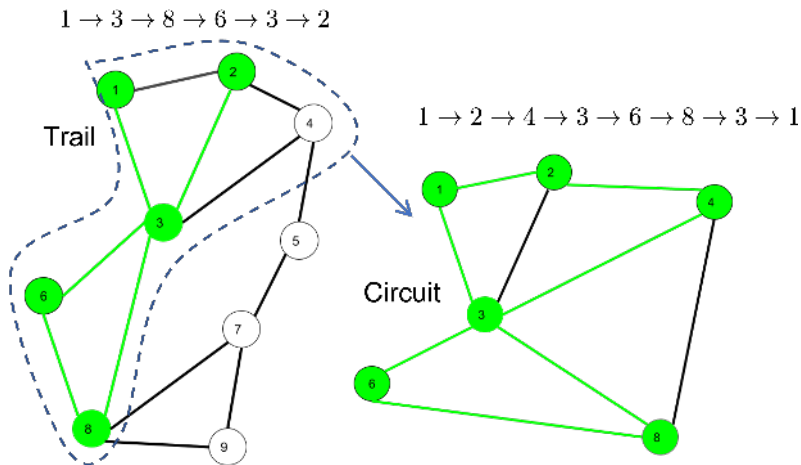
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Examples of trail and circuit





Path and cycle

Graphs topological characteristics

Path

A **path** between two nodes $p_{u,v}$ is a trail $t_{u,v}$ without repeated nodes.

Cycle

A **cycle** is a non-empty trail in which only the first and last vertices are equal and the edges are different too.

- For trees, forests and poly trees any walk that starts at the root or an internal nodes and ends to a leaf is a path.



Path and cycle

Graphs topological characteristics

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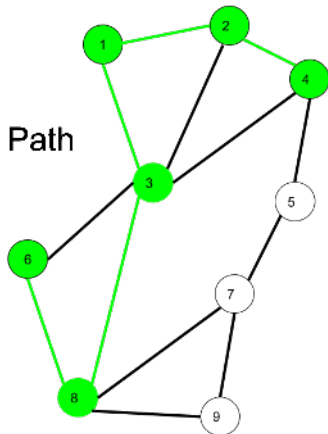
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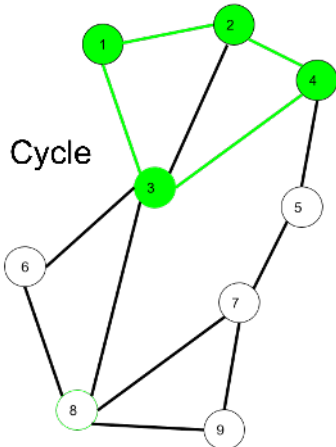


Examples of path and cycle

$$6 \rightarrow 8 \rightarrow 3 \rightarrow 1 \rightarrow 2 \rightarrow 4$$



$$1 \rightarrow 2 \rightarrow 4 \rightarrow 3 \rightarrow 1$$



Outline



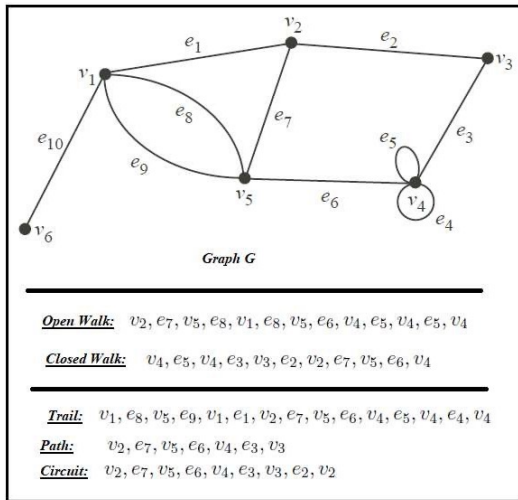
- 1 Walk, Trail, Path, Cycle
 - Distance between nodes



Distance on a graph

Graphs topological characteristics

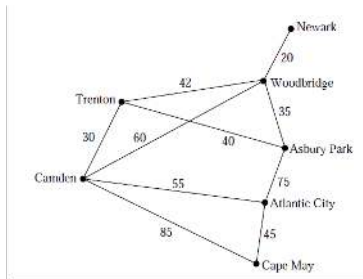
- The **graph distance** of two nodes is the length of the shortest path that connects them.
- The **path distance** for a weighted graph is $\sum_{e \in p_{uv}} w_e$ (is the edge weight).
- The **graph diameter** is the longest shortest path between any node pair.



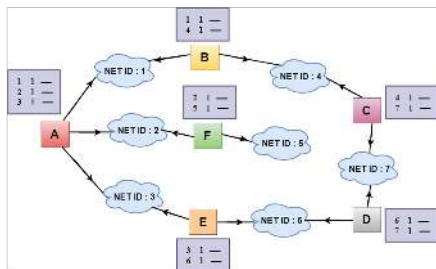


Why is this notion important?

- One of the most important features of a graph model is how difficult it is to reach its node from a certain origin
- It is important for flow networks, like routing or transportation



Transportation network



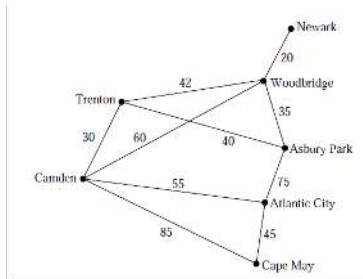
Communication network

- It is a feature that helps understanding how well connected the network is and correlates with fast graph dynamics.

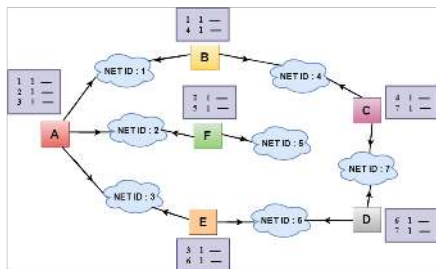


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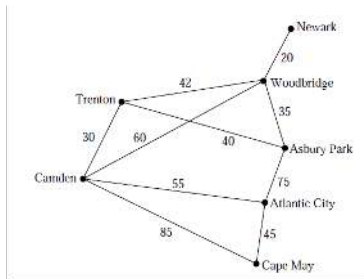
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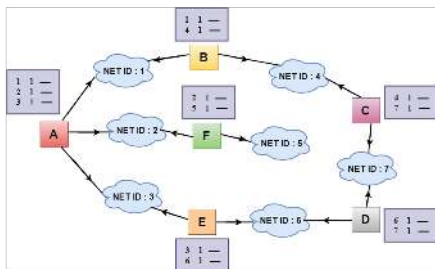


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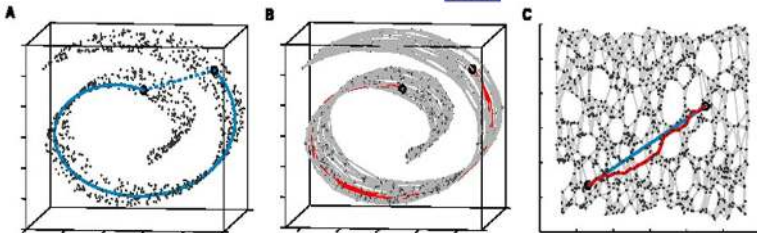
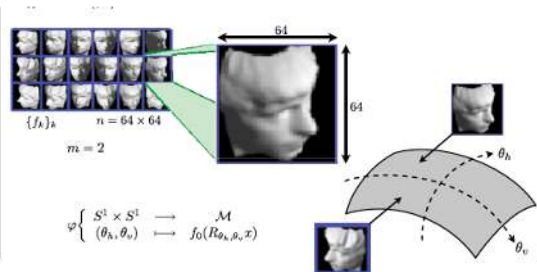
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Distance in graph representing data

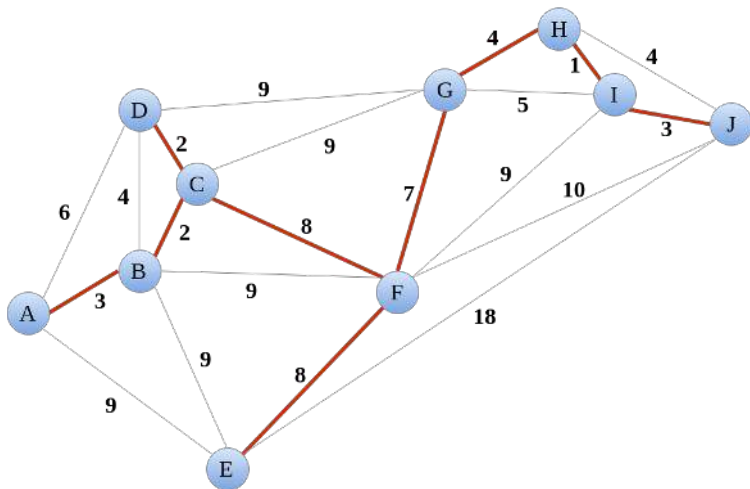
- We mentioned that graph can be a proxy to understand the low dimensional structure of data





Spanning Trees

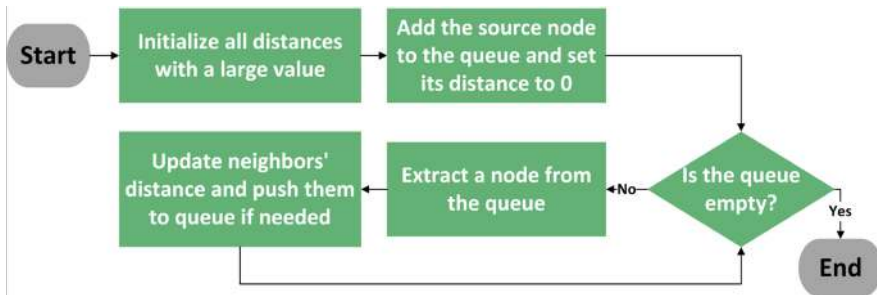
- A **spanning tree** connects all the vertices of a graph with the minimum possible number of edges. It is not unique in general.





Spanning Trees

- **Breadth First Search** or Dijkstra's algorithms find it with complexity $\Theta(|\mathcal{E}| + |\mathcal{V}|)$ or $\Theta(|\mathcal{E}| \log(|\mathcal{V}|) + |\mathcal{V}|)$. Dijkstra's alg. can minimize the sum of edge weights not just path lengths.





Networkx functions

In Networkx you can use the functions:

- `MINIMUM_SPANNING_TREE(G)` that uses Kruskal's algorithm to find a spanning tree from a certain source node.
- `SHORTEST_PATH(G)` which has the option of using Dijkstra or Bellman-Ford algorithms. It can use the weights, interpreted as edge distances/costs.
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Walks vs paths

- We will see that walks are easy to count algebraically using the adjacency matrix
- Paths are combinatorially hard (NP-hard variants appear quickly)
- This is why shortest paths calculations are algorithmic, not spectral

Outline



1 Walk, Trail, Path, Cycle

2 Algebra of networks

3 Conclusion

Outline



2 Algebra of networks

- Premise

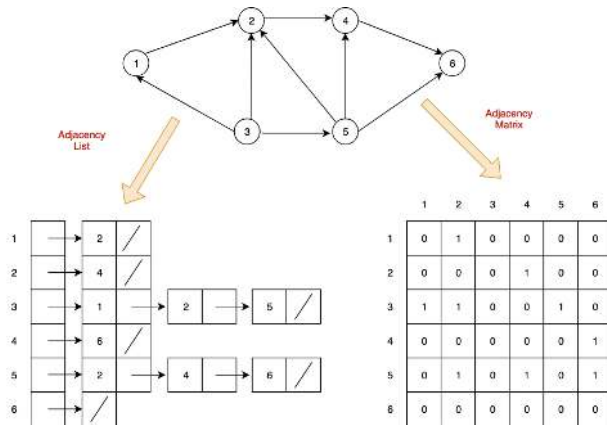
- Adjacency matrix



Premise

Algebra of networks

Matrices are not a compact representation of a graph when it is sparse. The adjacency list requires $O(|V| + |\mathcal{E}|)$ and the matrix $O(|V|^2)$.





Premise

Algebra of networks

- They are, however, very useful to understand how to model data that are explained by network dynamics, and inform algorithms to process them.
- They are also useful to explore the topology: Counting walks, measuring reachability, detecting communities, and modeling dynamics all reduce to matrix operations.
- Perhaps one of the most interesting is the Laplacian, which is used for various types of analyses (the study is called **spectral graph theory**)
- The Laplacian also emerges in a number of network dynamics and is fundamental in Graph Signal Processing.



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2 Algebra of networks

- Premise

- Adjacency matrix



Adjacency matrix

- The adjacency matrix $\mathbf{A}$ elements for a directed graph are:

$$A_{uv} = \begin{cases} 1 & \text{if there is an edge from } v \text{ to } u, \text{ i.e. } (v, u) \in \mathcal{E} \\ 0 & \text{else.} \end{cases}$$

- The definition above accounts only for the topology. The weighted adjacency matrix has elements:

$$A_{uv} = \begin{cases} w_{uv} & \text{if there is an edge from } v \text{ to } u \text{ with weight } w_{uv} \\ 0 & \text{else.} \end{cases}.$$

The diagonal terms are zero if the network has no self-loops.

- For undirected we need to add $A_{uv} = A_{vu}$, i.e. $\mathbf{A} = \mathbf{A}^\top$.
- **Note:** In `networkx` the adjacency generated is equal to $\mathbf{A}^\top$.

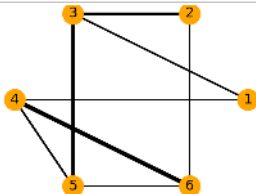
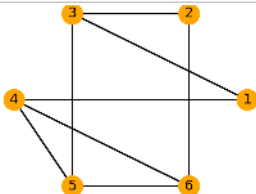
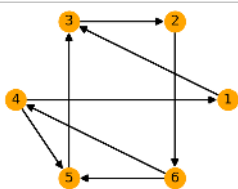
Visualization of different types of graphs



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

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$$\begin{bmatrix} 0. & 0. & 4.5 & 3.1 & 0. & 0. \\ 0. & 0. & 7.25 & 0. & 0. & 2.1 \\ 4.5 & 7.25 & 0. & 0. & 8.5 & 0. \\ 3.1 & 0. & 0. & 0. & 4.75 & 10.1 \\ 0. & 0. & 8.5 & 4.75 & 0. & 3.25 \\ 0. & 2.1 & 0. & 10.1 & 3.25 & 0. \end{bmatrix}$$



- On the left, a directed graph - note $\mathbf{A} \neq \mathbf{A}^\top$
- Middle and right side, undirected unweighted and weighted graphs



Degrees from the adjacency matrix

- Let $\mathbf{1}$ be the all ones vector. Note that for an unweighted and undirected graph/adjacency matrix the vector of degrees is $\mathbf{d} = \mathbf{A}\mathbf{1}$.
- For an unweighted directed graph
 - $\mathbf{d}^+ = \mathbf{A}\mathbf{1}$ is the vector of in-degrees $[d^+]_u = |\mathcal{N}_u^+|$.
 - $\mathbf{d}^- = \mathbf{1}^\top \mathbf{A}$ is the vector of out-degrees $[d^-]_u = |\mathcal{N}_u^-|$.
- Assuming that $\mathbf{A}$ is the weighted adjacency matrix, instead of the degrees the elements of $\mathbf{A}\mathbf{1}$ are the sums of the weights:

$$\sum_{v \in \mathcal{N}_u} w_{uv}$$



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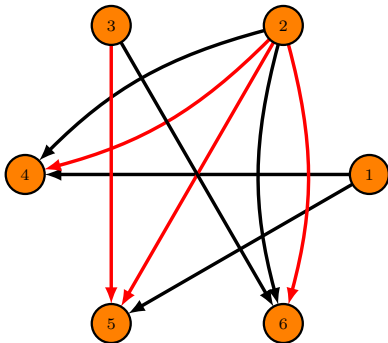


Adjacency matrix for multigraphs

- It is often better to look at the **multi-graphs** as a series of graphs $\mathcal{G}(t) = (\mathcal{V}, \mathcal{E}(t))$, but the convention used to define their adjacency matrix of a multi-graph is setting

$$A_{uv} = \text{number of edges from } v \text{ to } u \text{ in the set } \bigcup_{t=1}^T \mathcal{E}(t) = \sum_{t=1}^T A_{uv}(t).$$

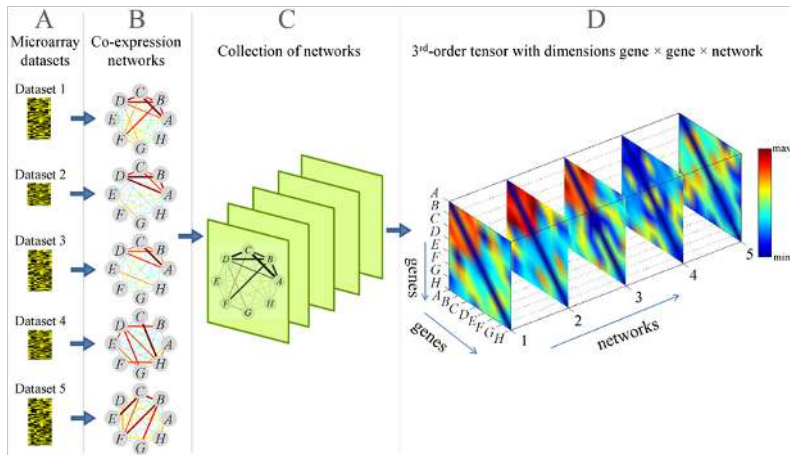
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Multigraphs adjacency tensor representation

A preferable representation is to consider a tensor $A_{uvt} = A_{uv}(t)$, whose *slices* are the matrices that correspond to the different graphs adjacency matrices, i.e. $\mathbf{A}_t : [\mathbf{A}_t]_{uv} = A_{uv}(t)$

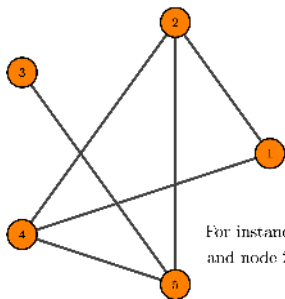




Number of walks

Number of walks

Consider a directed or undirected graph and a positive integer k . The number of directed and undirected walks respectively from node i to node j of length k is the entry on row i and column j of the matrix A^k , where A is the adjacency matrix.



$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{bmatrix}, \quad A^2 = \begin{bmatrix} 2 & 2 & 1 & 1 & 1 \\ 2 & 3 & 1 & 2 & 1 \\ 1 & 1 & 2 & 1 & 2 \\ 1 & 2 & 1 & 4 & 2 \\ 1 & 1 & 2 & 2 & 3 \end{bmatrix}, \quad A^3 = \begin{bmatrix} 2 & 3 & 3 & 6 & 5 \\ 3 & 4 & 5 & 7 & 7 \\ 3 & 5 & 2 & 6 & 3 \\ 6 & 7 & 6 & 6 & 7 \\ 5 & 7 & 3 & 7 & 4 \end{bmatrix}$$

For instance the element $[A^3]_{1,2} = 5$ is the number of walks between node 1 and node 2 of length 3. These walks are: $1 \rightarrow 4 \rightarrow 5 \rightarrow 2$, $1 \rightarrow 4 \rightarrow 1 \rightarrow 2$, $1 \rightarrow 2 \rightarrow 1 \rightarrow 2$, $1 \rightarrow 2 \rightarrow 4 \rightarrow 2$, $1 \rightarrow 2 \rightarrow 5 \rightarrow 2$



Connected graphs

Strongly connected graphs

If a graph is strongly connected then there exist a finite k , $1 \leq k \leq +\infty$ such that $\sum_{i=0}^k \mathbf{A}^i$ has all elements that are non-zero. For fully connected, clearly $k = 1$.

- In fact the elements of $\mathbf{A}^k$ are equal to the number of walks from any two nodes
- This is way larger than the number of paths



Graph Laplacian

- Another very important matrix for the analysis of both topological as well as graph data processes is **Laplacian matrix**. It is defined for undirected graphs as:

$$\mathbf{L} = \text{diag}(\mathbf{d}) - \mathbf{A}$$

- We will study this operator in detail. It measures how different are a node value from its neighbors

$$[\mathbf{L}\mathbf{x}]_i = \sum_{j \in \mathcal{N}_i} (x_i - x_j)$$

- We will see that if the Laplacian is never full rank. In fact, $\mathbf{L}\mathbf{1} = \mathbf{0}$. An undirected graph is strongly connected if the rank of $\mathbf{L}$ is $N - 1$.
- If the Laplacian has rank $N - k$ then there are k strongly connected components.
- These are results of *algebraic graph theory*.



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Graph Laplacian

- Another very important matrix for the analysis of both topological as well as graph data processes is **Laplacian matrix**. It is defined for undirected graphs as:

$$\mathbf{L} = \text{diag}(\mathbf{d}) - \mathbf{A}$$

- We will study this operator in detail. It measures how different are a node value from its neighbors

$$[\mathbf{L}\mathbf{x}]_i = \sum_{j \in \mathcal{N}_i} (x_i - x_j)$$

- We will see that if the Laplacian is never full rank. In fact, $\mathbf{L}\mathbf{1} = \mathbf{0}$. An undirected graph is strongly connected if the rank of $\mathbf{L}$ is $N - 1$.
- If the Laplacian has rank $N - k$ then there are k strongly connected components.
- These are results of *algebraic graph theory*.



Number of spanning trees

- There are two results on **the number of spanning trees** $t(\mathcal{G})$:

Cayley's formula

The number of spanning trees for the complete graph is n^{n-2} .

Kirchoff theorem

Let $\mathbf{L} = \text{diag}(\mathbf{d}) - \mathbf{A}$, where $\text{diag}(\mathbf{v})$ is a diagonal matrix with diagonal elements equal to v_i and $\mathbf{d}$ is the degree sequence. Then, denote by $\lambda_1, \lambda_2, \dots, \lambda_N$ are the eigenvalues of the matrix $\mathbf{L}$:

$$t(\mathcal{G}) = \frac{1}{|\mathcal{V}|} \lambda_1 \cdot \lambda_2 \dots \lambda_{N-1}$$

The Laplacian reveals many interesting properties for the corresponding graph and appears in many graph data models.

Outline



2 Algebra of networks

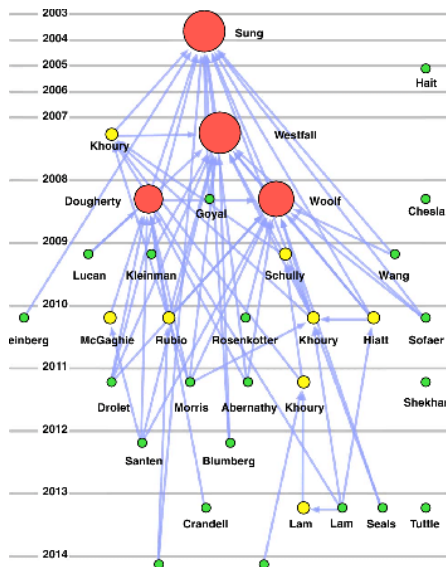
- Premise
- Adjacency matrix

Directed Acyclic Graphs (DAG): Example



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- Often, if the nodes are properly ordered, the matrix A reveals an underlying fact about the graph. DAG example: citation graphs.





Directed Acyclic Graphs (DAG)

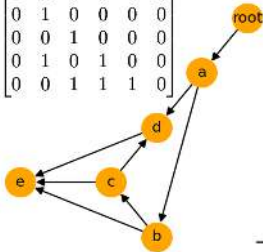
- One of such cases is that of DAGs, for which under proper ordering called *topological*, A appears as an upper triangular matrix.

Directed Acyclic Graph

Topological ordering

$\mathcal{V} = \{\text{root}, a, b, c, d, e\}$

0	0	0	0	0	0
1	0	0	0	0	0
0	1	0	0	0	0
0	0	1	0	0	0
0	1	0	1	0	0
0	0	1	1	1	0



Algorithm 1: Kahn's Algorithm for Topological Sort

Data: A DAG G

Result: A topological sort of all vertices in G

Compute in-degree (number of incoming edges) for each vertex in G ;

Put all the vertices with 0 in-degree into a queue Q ;

Create an empty vertex list L ;

while Q is not empty **do**

 Remove a vertex u from Q ;

 Add u to the end of the L ;

foreach u 's neighboring node v **do**

 Decrease v 's in-degree by 1;

if v 's in-degree is 0 **then**

 Add v to Q ;

end

end

end

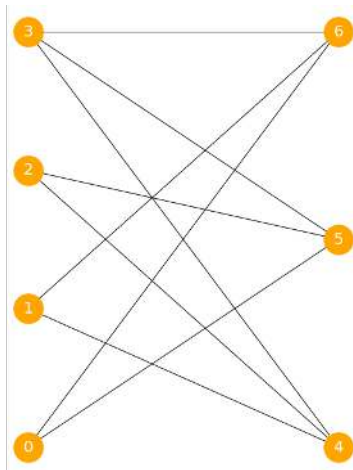
return L ;



Bipartite Graphs

- The adjacency matrix of bipartite graphs also has a natural order by placing the two groups together.

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

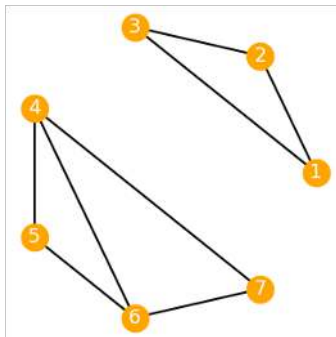




Disconnected Graphs

- The adjacency of a graph with disconnected component can also reveal the two communities. This graph is $\mathcal{G} = \mathcal{G}_1 \cup \mathcal{G}_2$

0	1	1	0	0	0	0	0
1	0	1	0	0	0	0	0
1	1	0	0	0	0	0	0
0	0	0	0	1	1	1	1
0	0	0	1	0	1	0	0
0	0	0	1	1	0	1	0
0	0	0	1	0	1	0	0



Outline



1 Walk, Trail, Path, Cycle

2 Algebra of networks

3 Conclusion



Concluding remarks

- We explored the properties of the adjacency matrix (completed in the next lecture)
- In the next lecture we will study the incidence matrix and its application to network flow problems.