



Lecture 2 - Graph topologies and characteristics

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

Anna Scaglione

Cornell Tech

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Content

- 1 Review
- 2 Graphs topological characteristics
 - Some graphs characteristics
 - Connectivity
 - Special types of graphs
 - Graph embeddings
- 3 Conclusions

Outline



- 1 Review
- 2 Graphs topological characteristics
- 3 Conclusions



Review and overview

- We introduced basic definitions that pertain graphs as well as graph structures.
- We rapidly surveyed a variety of models and examples that leverage graph based data science.
 - **Relational** interactions: social, economic, knowledge networks, biological.
 - **Data modeling networks** for deterministic multi-dimensional data or random observations.
 - **Networked** infrastructures: the internet electric power, transportation, gas, water, etc.
- Today we focus again on the study of graph structures and specific types of graphs



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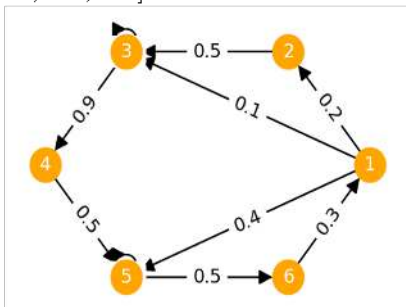
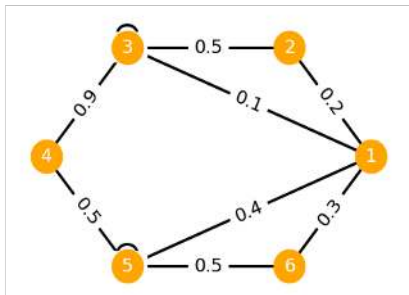


Definition of a graph

$$\mathcal{V} = \{1, 2, 3, 4, 5, 6\}$$

$$\mathcal{E} = \{(1, 2), (1, 5), (1, 3), (1, 6), (2, 3), (3, 3), (3, 4), (4, 5), (5, 5), (5, 6)\}$$

$$\begin{aligned} \mathbf{w} &= [w_{1,2}, w_{1,5}, w_{1,3}, w_{1,6}, w_{2,3}, w_{3,3}, w_{3,4}, w_{4,5}, w_{5,5}, w_{5,6}] \\ &= [0.2, 0.4, 0.1, 0.3, 0.5, 0.1, 0.9, 0.5, 0.5, 0.5] \end{aligned}$$



- We need to define the nodes, edge sets, possibly edge weights. For multigraphs we would have multiple sets of edges.



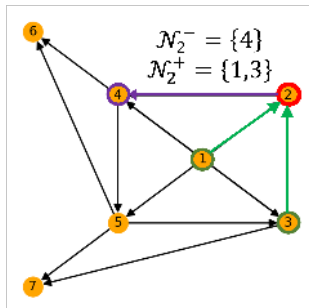
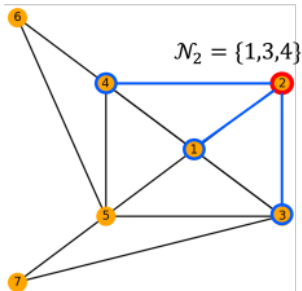
2 Graphs topological characteristics

- Some graphs characteristics
 - Connectivity
 - Special types of graphs
 - Graph embeddings



Neighborhoods

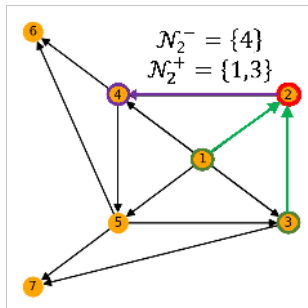
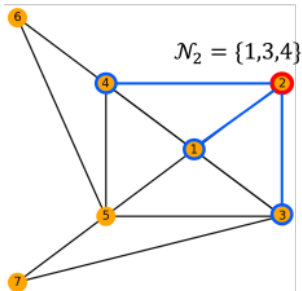
- $\mathcal{N}_v \subset \mathcal{V}$ contains all nodes connected to node v and the node degree $d_v = |\mathcal{N}_v|$
- $\mathcal{N}_v^+ \subset \mathcal{V}$ contains all nodes in edges that enter node, $\mathcal{N}_v^- \subset \mathcal{V}$ contains all nodes in edges that exit node v . In-degree and out-degree are $d_v^+ = |\mathcal{N}_v^+|$ and $d_v^- = |\mathcal{N}_v^-|$ respectively.





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Degree sequence

Graphs topological characteristics

The **degree sequence** is the vector $\mathbf{d} = [d_1, \dots, d_{|V|}]$ of nodal degrees. For directed graphs we have the sequence of in degrees and out degrees, $\mathbf{d}^+$ nad $\mathbf{d}^-$.

$$\mathbf{d} = [d_1, \dots, d_7]$$

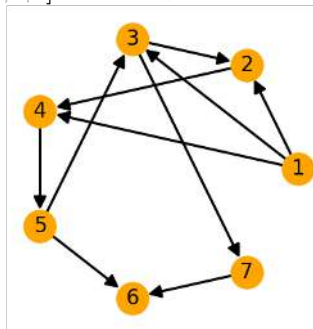
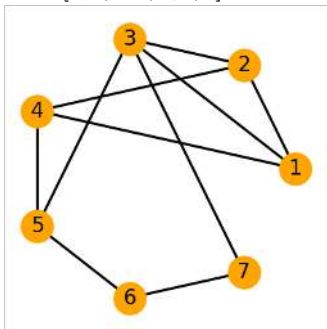
$$= [3, 3, 4, 3, 3, 2, 2]$$

$$\mathbf{d}^+ = [d_1^+, \dots, d_7^+]$$

$$= [0, 2, 2, 2, 1, 2, 1]$$

$$\mathbf{d}^- = [d_1^-, \dots, d_7^-]$$

$$= [3, 1, 2, 1, 2, 0, 1]$$





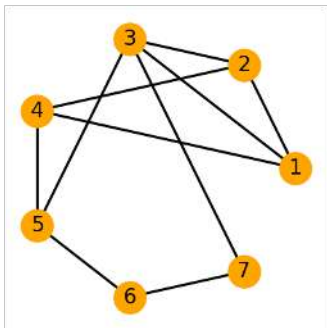
The average degree

Graphs topological characteristics

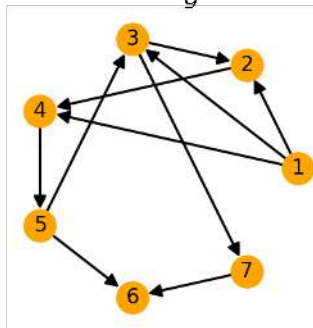
The **average degree** is:

$$\bar{d}_G = \frac{1}{|\mathcal{V}|} \sum_{v=1}^{|\mathcal{V}|} d_v, \quad \bar{d}_G^+ = \frac{1}{|\mathcal{V}|} \sum_{v=1}^{|\mathcal{V}|} d_v^+, \quad \bar{d}_G^- = \frac{1}{|\mathcal{V}|} \sum_{v=1}^{|\mathcal{V}|} d_v^-$$

$$d_G = 2.8571$$



$$\bar{d}_G^+ = 1.4285 \quad \bar{d}_G^- = 1.4285$$



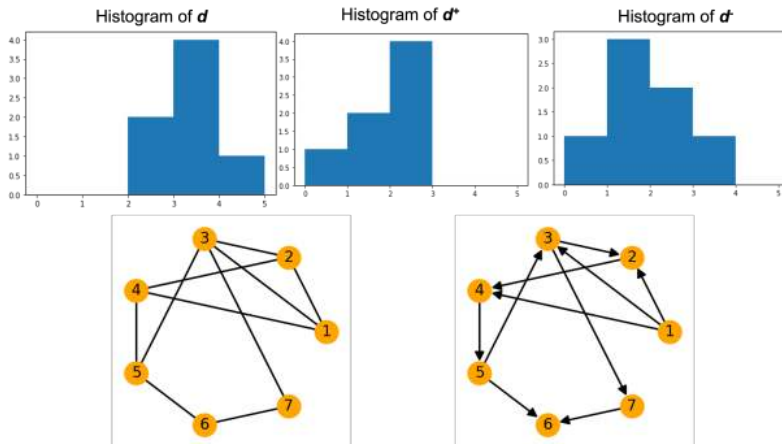


The empirical degree distribution

Graphs topological characteristics

The empirical **degree distribution** is the normalized histogram n_k :

$$P_{\text{degree}}(k) := \frac{n_k}{|\mathcal{V}|}, \quad n_k := \text{number of nodes with degree} = k$$





Network density

Graphs topological characteristics

- Let $|\mathcal{V}| = N$. If we don't consider self-loops the number of edges of an undirected graph is:

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

and for a directed graph is:

$$|\mathcal{E}| \leq N(N-1)$$

- Equality holds for a complete graph.

Network density

An undirected graph density is $\delta = \frac{2|\mathcal{E}|}{N(N-1)}$ and that of a directed graph is $\delta' = \frac{|\mathcal{E}|}{N(N-1)}$.



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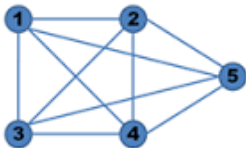


Sparse and dense networks

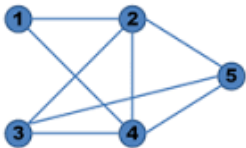
Graphs topological characteristics

- Many networks are relatively sparse.
- A tree is a sparse connected graph, and $|\mathcal{E}| = N - 1$.
- In general, a graph is considered **sparse** if the number of edges is $O(N)$ and dense if it is $O(N^2)$.

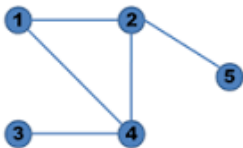
Complete Graph



Dense Graph



Sparse Graph



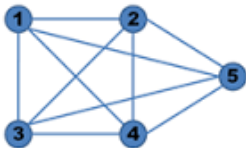


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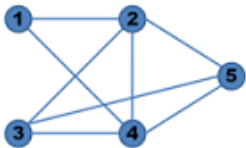
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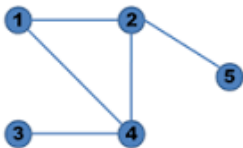
Complete Graph



Dense Graph



Sparse Graph



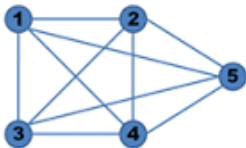


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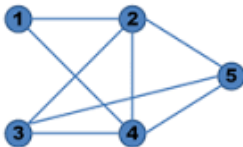
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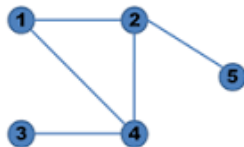
Complete Graph



Dense Graph



Sparse Graph





2 Graphs topological characteristics

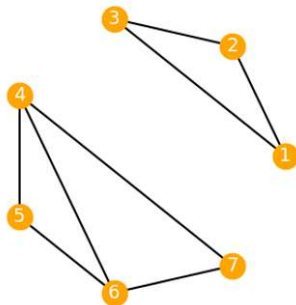
- Some graphs characteristics
- **Connectivity**
- Special types of graphs
- Graph embeddings



Disconnected graphs

- If a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is disconnected, we can divide the nodes into subsets of nodes that are strongly connected, forming a set of graphs $\mathcal{G}_k, k = 1, \dots, K$ that are called the **components** of $\mathcal{G}$.
- They are such that $\mathcal{V}_k \cap \mathcal{V}_{k'} = \emptyset$, $\mathcal{E}_k \cap \mathcal{E}_{k'} = \emptyset$ and:

$$\mathcal{V} = \bigcup_{k=1}^K \mathcal{V}_k, \quad \mathcal{E} = \bigcup_{k=1}^K \mathcal{E}_k$$



A graph with two components.

- Note that it is possible that some of these components are isolated nodes.
- A strongly connected graph is a **giant component**

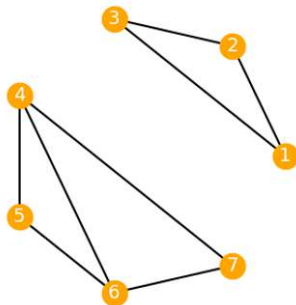


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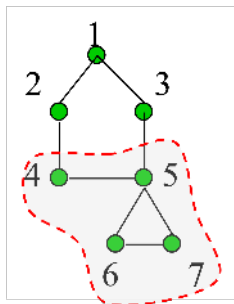
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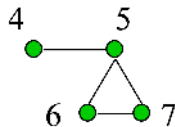
Subgraphs

Subgraph

A **subgraph** of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a graph whose nodes are a subset $\mathcal{V}_s \subset \mathcal{V}$ and whose edges $\mathcal{E}_s \subset \mathcal{E}$ are all edges connecting pairs of vertices in $\mathcal{V}_s$.



Subgraph

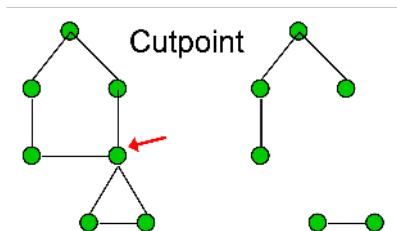




Cutpoints

Cutpoint

If removing a **vertex** from the graph and its edges to the rest of the network increases the number of **graph components** then such vertex is a **cutpoint**.

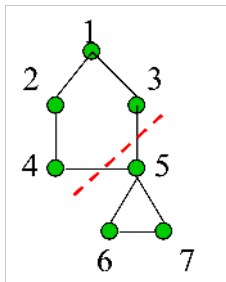




Network cuts

Network cut

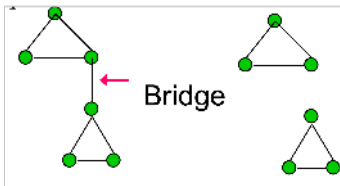
A **network cut** is a subset of edges $\mathcal{E}_{i,j} \subset \mathcal{E}$ such that removing those edges disconnects the network in two components with nodes respectively in $\mathcal{V}_i$ and $\mathcal{V}_j$ that form a partition of $\mathcal{V}$, i.e. $\mathcal{V}_i \cap \mathcal{V}_j = \emptyset$ and $\mathcal{V}_i \cup \mathcal{V}_j = \mathcal{V}$.



The cut is $\{(3,5), (4,5)\}$

Bridge

A **bridge** is a network cut that consists only of one edge.





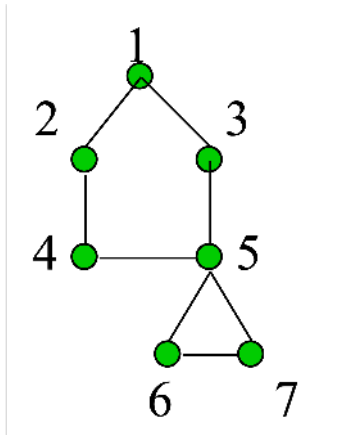
Connectivity

Vertex/Node Connectivity

The network **node connectivity** $\kappa(\mathcal{G})$ is the minimum number of nodes $\mathcal{V}$ whose removal disconnects the graph. A graph is **k-connected** if $\kappa(G) = k$.

Edge Connectivity

The network **connectivity** is the size of its minimum edge cut
 $\lambda(\mathcal{G}) := \min_{ij} \mathcal{E}_{i,j} \subset \mathcal{E}$ where the minimization is over all possible partitions of the nodes in two sets $\mathcal{V}_i \cap \mathcal{V}_j = \emptyset$.



$$\kappa(\mathcal{G}) = 1, \quad \lambda(\mathcal{G}) = 2$$



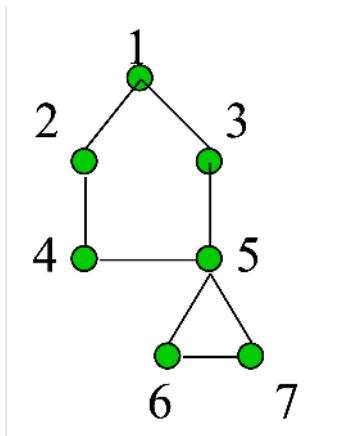
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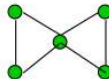
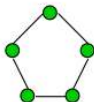
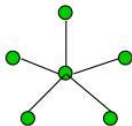


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Connectivity and edge connectivity

Graph



Edge-

Connectivity

1

2

2

4

Connectivity

1

2

1

4

Whitney's theorem

For any graph $\mathcal{G}$, $\kappa(\mathcal{G}) \leq \lambda(\mathcal{G}) \leq \delta(\kappa(\mathcal{G}))$, where $\delta(\kappa(\mathcal{G})) := \min_{v \in \mathcal{N}} d_v$ is the minimum degree in the graph.



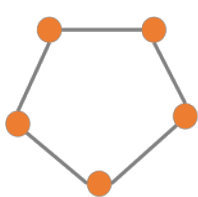
2 Graphs topological characteristics

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- **Special types of graphs**
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Specific families of graph topologies

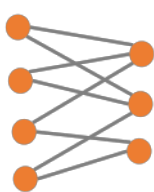
Graphs



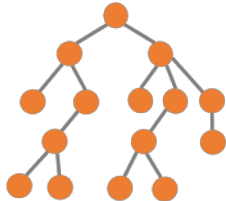
Cycle



Star



Bipartite



Tree

All these graphs can be directed or undirected (as shown).



Graphs without cycles

- We are going to talk more in the next lecture about the definitions of **path** in a graph and **cycles**.
- They are both quite intuitive: a path as a sequence of edges that are not repeated and that allow you to go from one node v to another node u in the graph through a series of intermediate edges (*hops*).
- A cycle is like a path but connects node v with itself.

Directed Acyclic Graph (DAG)

A directed graph with no cycles is a DAG.

- DAGs applications: biology (evolution, family trees, epidemiology), information science (citation networks), computation (scheduling tasks), learning (graphical models).



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Graphs without cycles (cont.)

Tree

A **tree** is an undirected graph in which any two vertices are connected by exactly one path, or equivalently a connected acyclic undirected graph.

Polytree

A **polytree** is a DAG whose underlying undirected topology is a tree.



Graphs without cycles (cont.)

Tree

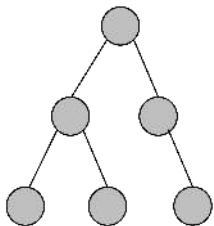
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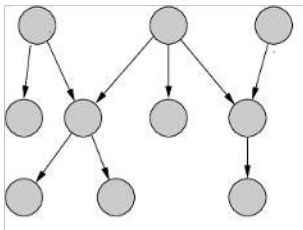
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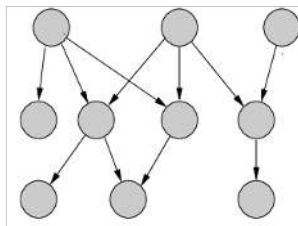
Graphs without cycles: examples



A Tree



A Polytree (also a DAG)



A DAG that is not a Polytree



Graphs without cycles

Forest

A **forest** is an undirected graph in which any two vertices are connected by at most one path. They are a disjoint union of trees.

Polyforest

A **polyforest** (or directed forest or oriented forest) is a directed acyclic graph whose underlying undirected graph is a forest.

Leaf

The **leaves** of a tree (polytree, forest, polyforest) are nodes with degree 1. Every other vertex v with $d_v > 1$ is internal.



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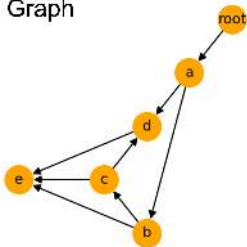
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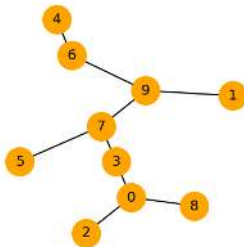


Examples

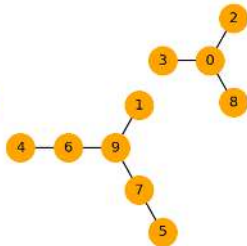
Directed Acyclic Graph



Tree



Forest



- To visualize DAGs is useful to apply what is called **topological sorting** of its nodes. The Networkx function is `NX.TOPOLOGICAL_SORT(GRAPH)`.

Topological sorting

A linear ordering of its vertices such that for every directed edge from vertex v to vertex u , v comes before u in the ordering.



Partial ordering for DAG

- Node v of a DAG is *reachable* from node u if there is a path connecting them.
- For DAG the topological ordering is associated to what is a **partial ordering** of the nodes that is based on reachability:

$$u \leq v \quad \Leftrightarrow \quad \text{if } v \text{ is reachable from } u$$

- The partial ordering is not *one to one*, in the sense that multiple DAGs can lead to the same partial ordering of a set of nodes.
- A **topological ordering** of nodes into a sequence is such that for every edge the start node of the edge occurs earlier than the end node of the edge. It is possible only for DAGs



Properties of trees

- Trees are such that $|\mathcal{E}| = |\mathcal{V}| - 1$. The condition $|\mathcal{E}| \geq |\mathcal{V}|$ is the simplest check to determine if an undirected graph has cycles!
- For a forest, we can count the number of trees n_{tree} since $|\mathcal{E}| = |\mathcal{V}| - n_{\text{tree}}$
- In a rooted tree, one internal node is designated as the root. The **height** or **depth** of a rooted tree, is the maximum path length from root to leaf.



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Combinatorial studies: Ex. Number of trees

- For most families of graphs someone has attempted to calculate how many possible different graphs of that type exist. These are typically some special combination.
- They can be useful when reasoning on random graphs.

Number of possible trees

The number of trees whose nodes have a specific tuple of degrees $\mathbf{d} = (d_1, \dots, d_{|V|})$ is the multinomial coefficient:

$$\kappa(\mathbf{d}) = \binom{n-2}{d_1-1, d_2-1, \dots, d_{|V|}-1}$$

- Modeling trees as the outcome of a random experiment, then $1/\kappa(\mathbf{d})$ can be considered as the *probability* of a certain tree with degrees $\mathbf{d}$.



Bipartite Graphs

Bipartite Graph

A Bipartite Graphs (a.k.a. Bigraph) is a graph whose vertices can be divided into two disjoint and independent sets $\mathcal{A}$ and $\mathcal{B}$, called the *parts of the graph* $\mathcal{G}$, so that every edge $e \in \mathcal{E}$ is $e = (a, b)$, $a \in \mathcal{A}$, $b \in \mathcal{B}$. A *balanced* Bipartite Graph has $|\mathcal{A}| = |\mathcal{B}|$.

- A graph is bipartite if and only if it does not contain an odd cycle. Trees are bipartite graphs (...it has no cycles at all!)
- The algorithm Depth First Search (DFS) can be used to verify if the graph is bipartite.



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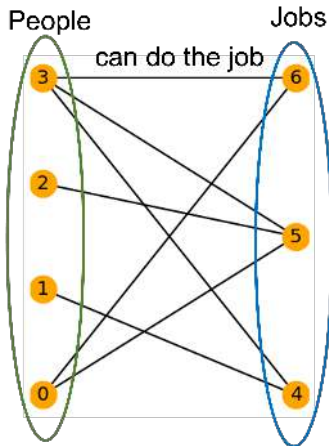
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Bipartite Graphs models

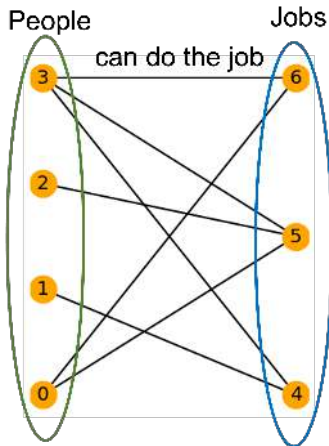
- Bipartite graphs are good models for *group membership*
- For example: suppose we have a set of people and set of jobs. Each person can do only some of the jobs.
- A bipartite graph that connects people with jobs is a natural representation.





Bipartite Graphs models

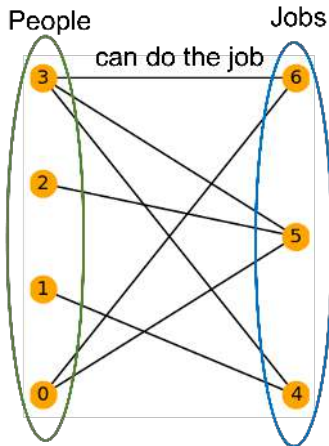
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Nodal degrees properties

Degrees and edges

For a general undirected graph:

$$\text{Handshaking theorem} \quad \sum_{v \in \mathcal{V}} d_v = 2|\mathcal{E}|$$

The proof is simple $\sum_{v \in \mathcal{V}} d_v = |\bigcup_{v \in \mathcal{V}} \mathcal{N}_v|$ in which each edge (u, v) is counted twice.

Degrees and edges of a bipartite graph

For a bigraph:

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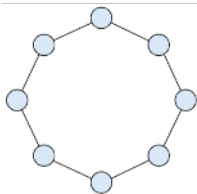
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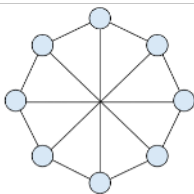
Regular graphs

The d -regular graph

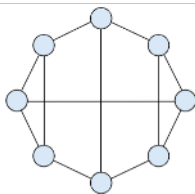
In a d -regular graph every node has the same degree d .



2-regular



3-regular



3-regular

Regular tree

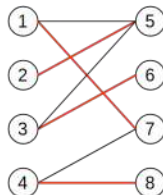
In a d -regular tree all internal nodes have the same degree.



Balanced graphs

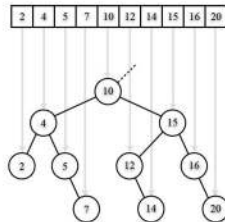
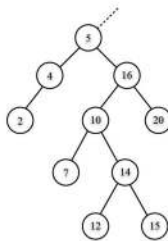
Balanced bipartite graph

A *balanced* bipartite graph has $|\mathcal{A}| = |\mathcal{B}|$.



Balanced tree

In a height-balanced tree the left and right subtrees height of any node differs at most by one.





2 Graphs topological characteristics

- Some graphs characteristics
- Connectivity
- Special types of graphs
- **Graph embeddings**



Embedding graphs on surfaces

Graph embeddings

A graph $\mathcal{G}$ embedding is a representation of the graph nodes as points and its edges as arcs on a surface $\mathcal{S}$ such that:

- 1 The vertexes $v \in \mathcal{V}$ are distinct points $x_v \in \mathcal{S}$
- 2 Edges $(u, v) = e \in \mathcal{E}$ are arcs/curves on the surface $\mathcal{S}$ whose end-points are x_u and x_v .
- 3 The arcs cannot intersect with other arcs, or include points associated with other vertexes.

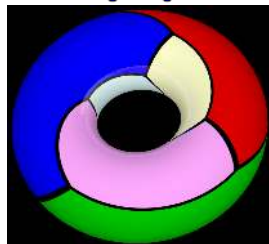
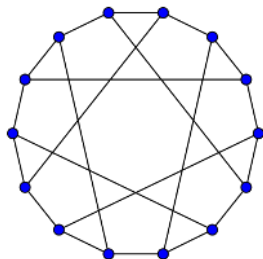
Note:

- An *embedding* asks whether the graph can be drawn on a surface with *no* edge crossings (except at common endpoints).



Embedding graphs on surfaces

- Note that a *drawing* of a graph in the plane may have crossings *even if* the graph is planar (see right).
- If the embedding is possible the complement of the graph is the disjoint union of connected components called *faces* and are simply connected (can be deformed into a disk).
- On the right, the Heawood graph and the associated map embedded in the torus.



Key takeaway

Planarity is a property of the abstract graph, not of a particular picture.



What changes, what doesn't

Topology mindset (informal)

Topology studies properties preserved under continuous deformations: *stretching* and *bending* are allowed, but *tearing* and *gluing* are not.

Combinatorial / graph invariants

- adjacency and degree sequence
- connected components
- existence of cycles (odd/even cycles)
- cuts, bridges, vertex/edge connectivity

Not invariants (depend on the drawing)

- lengths / angles of edges
- the apparent “shape” of the drawing
- whether edges cross *in that drawing*



Planar graphs

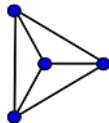
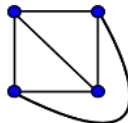
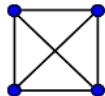
Planar graphs

A planar graph is a graph that can be embedded in the plane drawn in a way that no edges cross each other.

Euler's theorem

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a connected planar graph, and let $\mathcal{F}$ be the set of faces of $\mathcal{G}$ in a planar embedding. Then,

$$|\mathcal{V}| - |\mathcal{E}| + |\mathcal{F}| = 2$$





Genus: how much “surface” a graph needs

- Some graphs are *not* planar: they cannot be embedded in the plane without crossings.
- If we allow a more complex surface (e.g., a torus), some non-planar graphs become embeddable.

Genus (informal definition)

The *genus* g of a surface is the number of “handles”. The *genus of a graph* is the minimum g such that the graph can be embedded on a surface of genus g without crossings.



Genus Theorem

Euler characteristic (orientable surfaces)

If a graph $G = (V, E)$ is embedded on an orientable surface of genus g with face set F , then

$$|V| - |E| + |F| = 2 - 2g.$$

- Plane / sphere: $g = 0 \Rightarrow |V| - |E| + |F| = 2$ (your planar Euler formula)
- Torus: $g = 1 \Rightarrow |V| - |E| + |F| = 0$



Two notions of “embedding” in graph data science

(A) Graph $\rightarrow$ surface

- nodes $\mapsto$ points on a surface
- edges $\mapsto$ non-intersecting arcs
- yields faces, planarity, genus
- **Goal:** respect topology (no crossings)

(B) Graph $\rightarrow \mathbb{R}^d$

- nodes $\mapsto$ vectors in $\mathbb{R}^d$
- geometry reflects similarity/diffusion (Laplacian eigenmaps, node2vec, GNN embeddings...)
- **Goal:** *create a geometry for learning*

Punchline

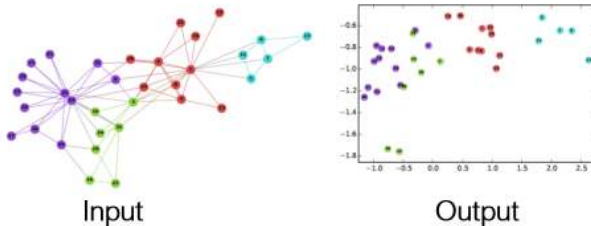
One embedding respects topology; the other produces geometry.

- (A) In this lecture we connected graph theory with topology (faces, planarity, genus).



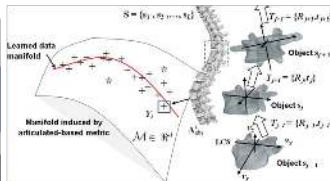
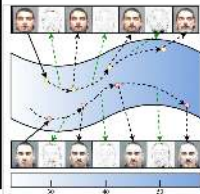
Example of graph embedding

- The graph is converted in a set of points in $\mathbb{R}^d$ that is not necessarily over a surface and that is an encoding of its nodes
- It will be discussed later in the course...

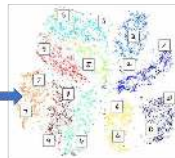


Continuous data topology converted into graphs

- This notion is used when graphs formed with data $x_i \in \mathbb{R}^d$ $d > 1$ that are proxies for manifolds of dimension $d' < d$ containing the data. Think about point clouds for example.
- Meshes are graph representations of complex objects (e.g. faces).



Manifold Learning



Outline



- 1 Review
- 2 Graphs topological characteristics
- 3 Conclusions**



Concluding remarks

- In this lecture we introduced a number of definitions and type of graphs that will be useful as models for real networks.
- We will leverage these definitions in the study algebraic methods to characterize graphs.
- In this first phase, the data we are interested in analyzing are the graphs themselves and their properties.