Lecture 1 - Introduction

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

Anna Scaglione

Cornell Tech

January 21, 2026

Content

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Outline

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People

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Information about the course

Instruction Schedule

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- **Office hours** (they are after class): TA and/or Instructor
  – Time 4:15 pm to 5:15pm (Bloomberg 216)
- Office hours meetings are in person. You have to send us an email/slack message prior to let us know, so that we best use that time slot.
- There is **slack channel** for this course, you can see the link on the Syllabus to join on Canvas. It is great for short questions. If you ask them under a common channel everyone can read the reply, so it is much better.
- The **lecture slides** will be made available after the lecture (due to possible corrections) on Canvas under **Modules**.

Information about the course

Testing

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The following home assignments will determine your grade.

- The calendar indicates the days in which homework is assigned and when it is due.
- The **two midterms** that are small projects and they are also submitted online, they take two weeks.
- There is **final assignment** that is also a project. This will be a team project and you pick a relevant graph data topic to work on. I will ask you in the midterm questions on the plan for your team and topic.

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Assignments description

Testing Etiquette

- Homework is assigned on Wednesdays and due the Thursday of the following week
- There will be some basic theory tested and require using Python.
- On the day of the assignment the theory will be mostly tested through a short quiz in class
- For the rest of the homework you can use AI chatbots, but you have to document the discussion with the chatbot and provide comments.
- Answers and code with no explanation, code that does not run, does not produce output tables/figures will be give a grade of 1 for participation.
- **New**– Pop-up oral exam sessions on the homework that the students return will be integrated in the lectures.

Information about the course

Testing

Warnings:

- We use **Gradescope** for the assignments and for grading
- Quizes are pen and paper, we collect them and grade them
- Assignments posted online are returned on Canvas electronically (follow the instructions).
- **Late submissions**: I will detract 5% for the first day and increase this detraction by 10% each day of delay after the first for up to 3 days.
- The **grades** assigned will be typically on a scale from 0 to 4 and then the average are rescaled between 0 and 100 to give you the letter grade.

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Information about the course

Your health and wellbeing matters!

Cornell University

- We love to help. Studying requires effort, and we get it.
- Please give us feedback and communicate early and often with us to let us know how we are doing.
- But, please, also be respectful of our time too and try to stick to the scheduled times unless it is important.

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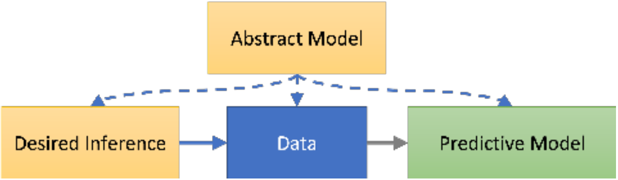

- **Why models?**: Could we not just use training data?
- Network model abstractions help formulate inference problems and help overcome the shortage/lack of training data
- For signals justified by a graph support we will see that extracting features can leverage the graph structure.

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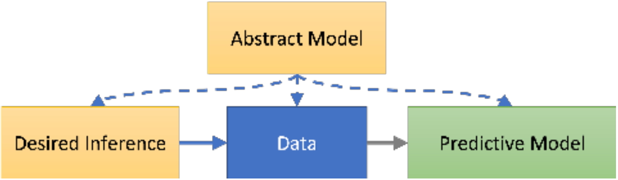

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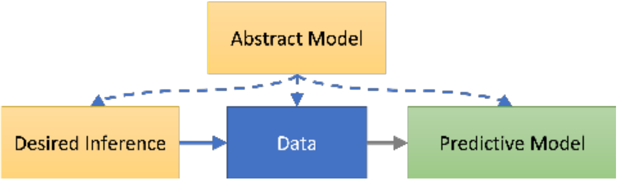

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First objective: modeling

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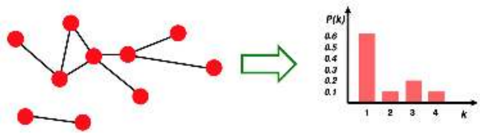
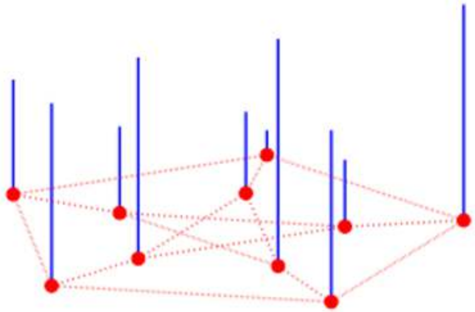
- Complex Network Systems and Graph models



- Data Associated to Networks



Second objective: data analysis

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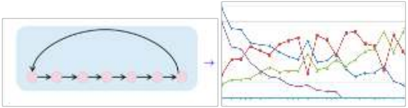
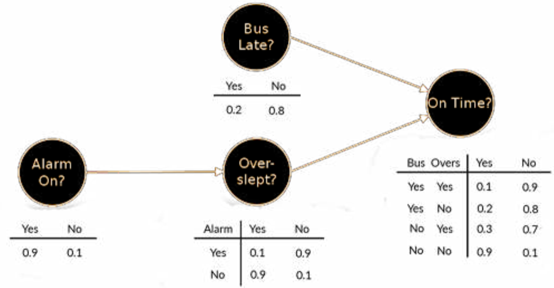
- Graph Topology Data Analysis: analyze the graph itself
- Graph Signal Processing: analyze data indexed by a network



Data indexed by time

Data indexed by a graph

- Bayesian Networks: to leverage conditional independence encoded in a network for statistical inference



Outline

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Complex Networked Systems

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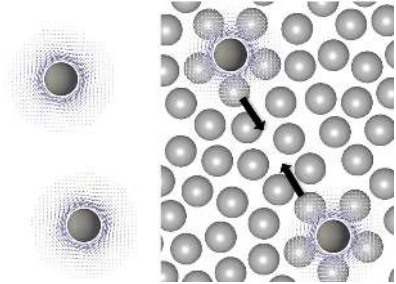
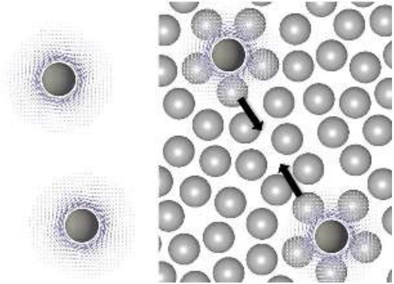


- *Complex Networked Systems* (CNS) studies seek a unified theory to interpret various phenomena by analyzing graph models to predict emergent behavior.
- Statistical physicists coined the name of CNS, and borrowed models from the study of interactive particles.
- CNS analysis is the subject of intense studies in data science.

Complex Networked Systems



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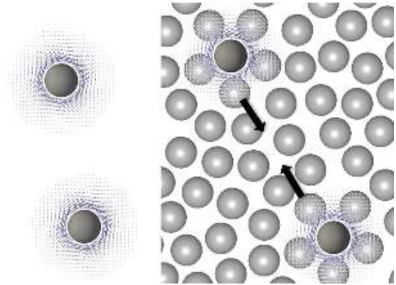

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Definitions

Graphs

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- Graphs $\mathcal{G} = (\mathcal{V}, \mathcal{E})$:
  - $\mathcal{V}$ is a set of nodes or vertices,
  - $\mathcal{E}$ is a subset of $\mathcal{V} \times \mathcal{V}$ that are links/edges connecting pairs of nodes (u, v).
- Undirected Graphs: edges are bidirectional, i.e. if $(u, v) \in \mathcal{E}$, then $(v, u) \in \mathcal{E}$.
- Directed Graphs: edge can, but do not have to be bidirectional. The edge (u, v) is from v to u.
- Multi-Graphs: nodes can have multiple edges (called parallel edges) connecting them. In CNS Multiplex Networks are a special case.

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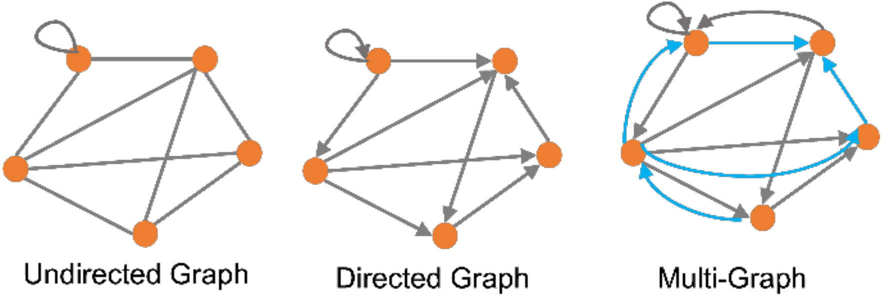
Different types of graphs

Graphs



Connectivity

A complete graph has all pairs of nodes connected by an edge. A strongly connected network has a path that connects every pair of nodes.

Line Graph

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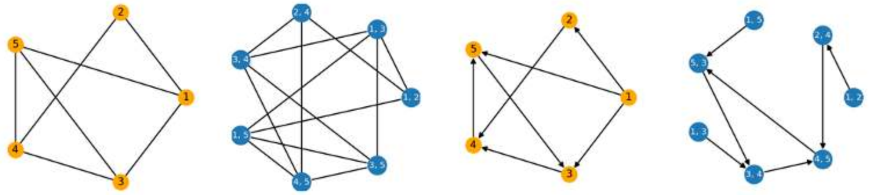
For a given graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, its line graph $\mathcal{L}(\mathcal{G}) = (\mathcal{V}', \mathcal{E}')$ is a graph such that:

- each vertex of $L(\mathcal{G})$ in an edge of $\mathcal{G}$, i.e. $\mathcal{V}' = \mathcal{E}$;
- two vertices of $L(\mathcal{G})$ are adjacent if and only if their corresponding edges share a common endpoint ("are incident") in $\mathcal{G}$, i.e. $\mathcal{E}' = \{(e, e')|e = (u, v), e' = (v, v'), u, v \in \mathcal{V}, e, e' \in \mathcal{E}\}$

That is, it is the *intersection graph* of the edges of $\mathcal{G}$, representing each edge by the set of its two endpoints.



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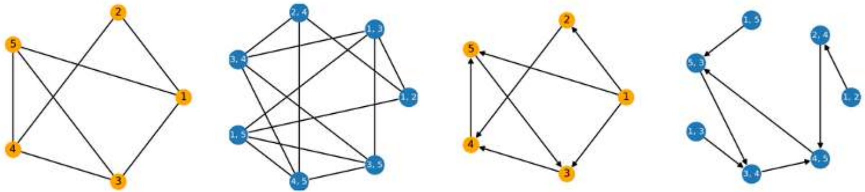

Generalization: Hypergraphs

Graphs

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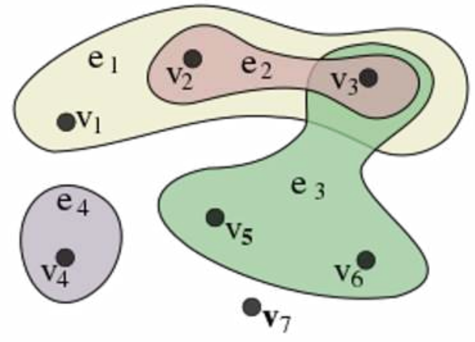
- In a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ the set of edges is $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$.
- Hypergraphs generalize the notion of graph, where $\mathcal{E}$ is a collection of subsets of $\mathcal{V}$.
- Technically, $\mathcal{E}$ is a subset of the *power set* of $\mathcal{V}$ (i.e. the set of all possible subsets formed with the elements of $\mathcal{V}$)



Affiliation networks are technically hypergraphs. On the other hand it is often better to map the network into a bipartite graph (defined soon).

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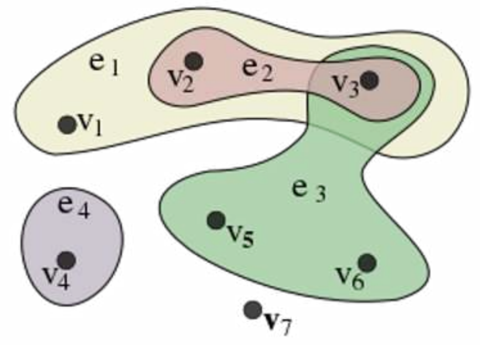

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Graph representation fundamentals

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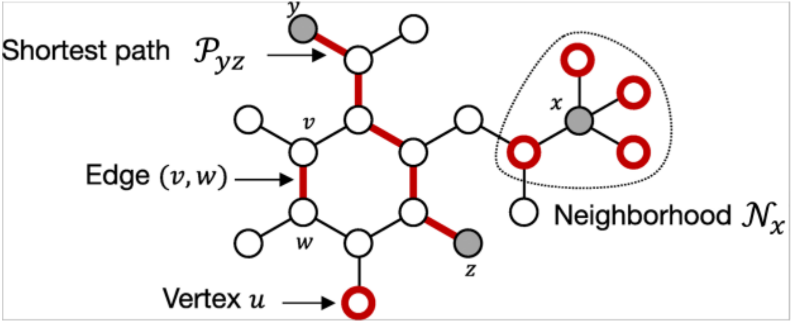

The edges and vertices highlighted illustrate specific definitions:

- The neighborhood $\mathcal{N}_x$ of a vertex x is the set of vertices connected to x by an edge.
- The path $\mathfrak{p}_{y,z}$ also happens to be the shortest path (sequence of vertices) between vertices y and z in this graph.

Graph representation fundamentals

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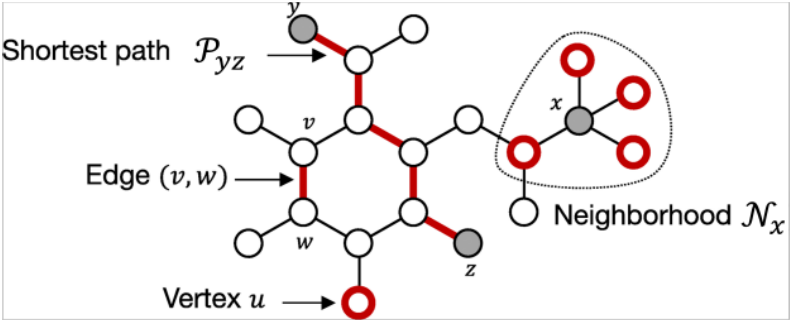

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Neighborhoods: undirected graph

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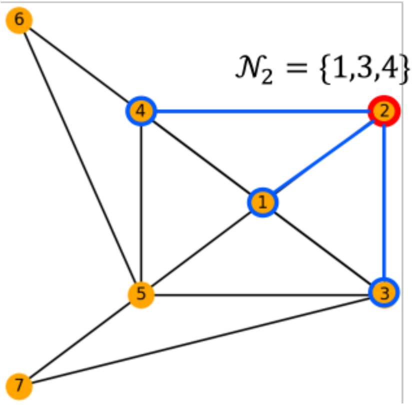
- For each node $v \in \mathcal{V}$ of an undirected graph the neighborhood subset $\mathcal{N}_v \subset \mathcal{V}$ contains all nodes connected to node v.

- The node degree $d_v = |\mathcal{N}_v|^1$ is the number of nodes in $\mathcal{N}_v$.



[1] $|\mathcal{A}|$ denotes the number of elements in the set $\mathcal{A}$ (its cardinality).

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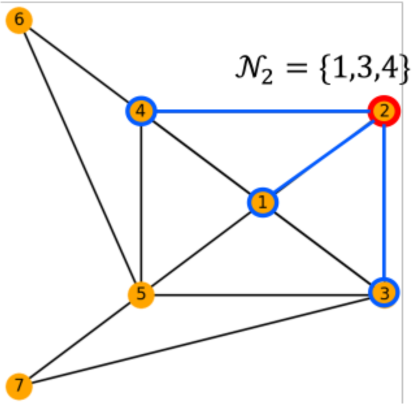

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Neighborhoods: directed graph

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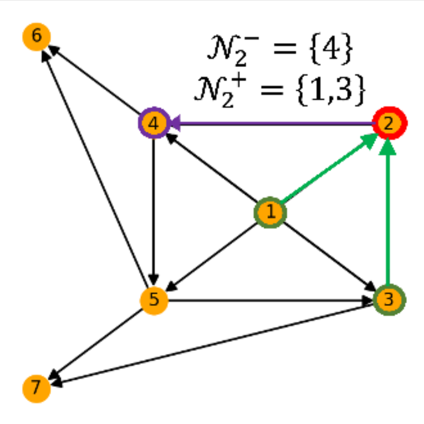
For each node $v \in \mathcal{V}$"

- the in-neighbohood subset $\mathcal{N}_v^+ \subset \mathcal{V}$ contains all nodes in edges that enter node v (a.k.a. *predecessors*), and $d_v^+ = |\mathcal{N}_v^+|$ is the in-degree
- the out-neighbohood subset $\mathcal{N}_v^- \subset \mathcal{V}$ contains all nodes in edges that exit node v (a.k.a. *successors*), and $d_v^- = |\mathcal{N}_v^+|$ is called the out-degree



What are $\mathcal{N}_1^-$ and $\mathcal{N}_1^+$?

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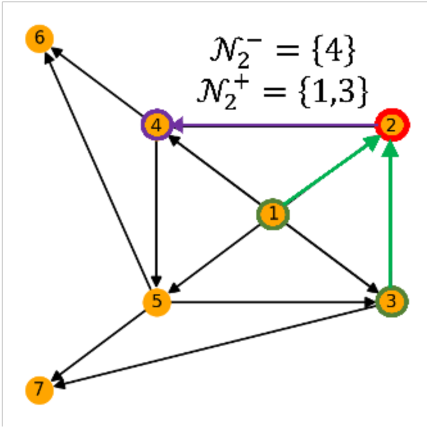

What are $\mathcal{N}_1^-$ and $\mathcal{N}_1^+$?

Attributes

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- $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is the topology, i.e. the scaffold of the network.
- Possible attributes and data associated to graph models:
  1. *edge weights* $w_{uv}, \forall (u,v) \in \mathcal{E}$, possibly time varying, i.e. $w_{uv}(t)$ where t is time . They are often positive and express the relative *strength* of the relationship.
  2. an edge flow $f_{uv}, \forall (u,v) \in \mathcal{E}$
     - Flow networks $(\mathcal{G}, \overline{f}, s, d)$ are directed graphs with a flow upper-limit $f_{uv} \leq \overline{f}_{uv}$ called the capacity function and two special nodes called source and sink/target/destination (s, d).
  3. a nodal graph signal $x_v, \forall v \in \mathcal{V}$, which may or may not be tied to explicit edge flows.
  4. edge labels l_{uv}, defining a relationship of nodes (u, v).
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Randomness and dynamics

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- Random graphs: Given a set of nodes $\mathcal{V}$ the topology of a random graph is the result of a random experiment whose outcome is the edge set $\mathcal{E}$.
- Dynamic graphs: Change topology in time $\rightarrow \ \mathcal{G}(t) = (\mathcal{V}(t), \mathcal{E}(t))$, possibly at random.
  - It can be modeled as a change in the weights $w_{uv}(t)$, that make the adjacency matrix dynamic $\boldsymbol{A}(t)$
- Graphs nodal dynamics: they refer to the temporal dynamics of nodal signals $x_v(t)$ and edge flows $f_{uv}(t)$, which can be stochastic processes or follow deterministic dynamical equations.

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Outline

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1. Information about the course
2. Introduction to the course
3. Graphs: basic definitions
4. Python tools for networks analysis
5. Examples of complex networks
6. Conclusion

Python for analyzing graphs

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- NetworkX Quite easy to use, very well documented, maybe you are already familiar with it. A lot of predefined function that facilitate the analysis of graphs.
- There are basic visualization functions, but better tools are available.
- There are function to derive the matrix representations (Adjacency, Incidence matrix, Laplacian and more) listed in the tutorial NetworkX and Numpy.

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Outline

Data from models conceptualized as a network

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Examples

- **Relational** interactions: social, economic, knowledge networks, biological
- **Data**: They are multi-dimensional data indexed by the nodes and can be random.
- **Networked** infrastructures: the internet electric power, transportation, gas, water, etc.

Network science

Task 1: mapping them into a network structure mathematically as a graph with attributes. **Task 2**: develop a model for the data, such as nodal and edge attributes (like signals and flows).

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Relational networks

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- In this categories we find networks that model human activities that are affected by mutual interactions: social, economic and collaboration networks,
- We can place in this class also biological networks, that are model biochemical processes, neurons interactions, but also swarms and interactions of different complex organisms
- The other important class of relational networks comes from *information science*, such as knowledge networks.
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Graphical models or Bayesian Networs

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- Here the node labels are random variables. The edges?
- **Bayes' law of probability** states that $P(Y|X) = P(Y \cap X)/P(X)$, i.e. the probability of an event or outcome Y given that I know that X has a certain outcome equals the probability of both happening together ($\cap$ means AND) normalized by the probability of the outcome for X.
- If $P(Y|X) = P(Y)$, then X and Y are **independent**. Knowing X does not change how uncertain you are about Y. **These nodes are disconnected.**
- When $P(Y|X) \neq P(Y)$ then they are connected but could be that there is a path in the network through another random variable due to conditional independence:

$$P(Y|X, Z) = P(Y|Z), \quad X \to Z \to Y$$

Graphical models or Bayesian Networs

- Graphical models are also relational network and are very general: they express conditional independence assumptions between random variables or events for any phenomenon.
- Conditional independence between random variables/events is expressed as follows. Z is **conditionally independent** on X given Y iff:

$$X \to Y \to Z \quad \Leftrightarrow \quad P(Z|Y,X) = P(Z|Y)$$

- In words, if you know Y happened, or its outcome, what outcome occurred for X does not matter as far as the probability distribution of Z is concerned.
- Note that if you do not know Y then in general $P(Z|X) \neq P(Z)$

Social and economics networks

Examples

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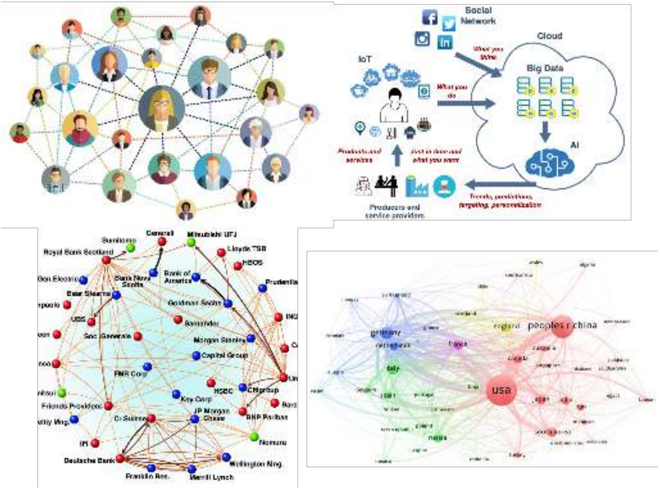

- Social, financial, collaboration..

Social and economics networks
Examples

- **Social networks** attracted interest since the 18^{th} century, even fostering the idea of democracy ("The wisdom of the crowds"). Later studies on *opinion dynamics* revealed a less rosy picture (i.e. polarization or herding)
  - Past sources of data were *surveys*. Nowadays an abundance of data comes from social platforms.
- **Economic networks** are intensely studied in investment firms, to predict markets trends.
  - Quarterly reports of financial activities provide the hard data.
  - Stock markets are shaped by the beliefs of the investors (like opinions in social networks).
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Information networks
Examples

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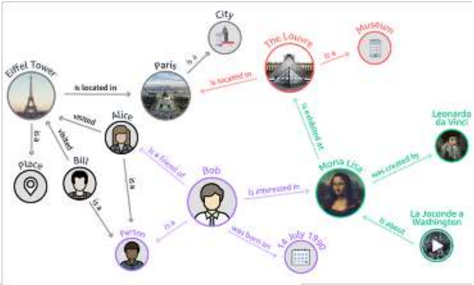

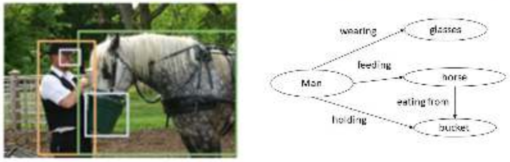

Figure 7: A knowledge graph created using computer vision techniques of object and edge detection

- websites hyperlinks networks, knowledge network, ontologies

Information networks
Examples

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- **Hyperlinks networks**: a directed network linking documents or different parts of one document. The subject of hyperlink network analysis (HNA) and Webometrics
  - In HTML Hypertext REFerence (href) linking webpages and URI of other target documents
  - Example of Webometrics: the algorithm PageRank
- **Knowledge networks**: representations of entity relations
  - Data come from model representation techniques such as:
    - Ontologies (on the Internet represented by the Web Language (OWL)): *class* → *attributes* → *relations*, etc.. Ontologies are domain dependent.
    - The Resource Description Framework (RDF) a standard to encode a statement structure as *subject* → *predicate* → *object*.
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Networks in biology

Examples

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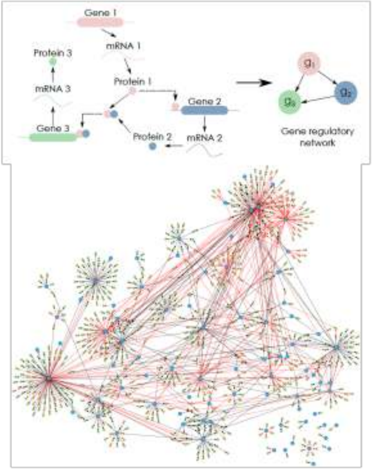
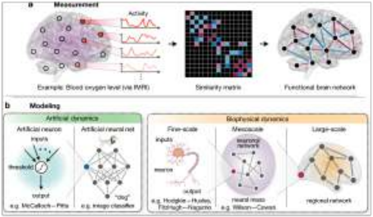
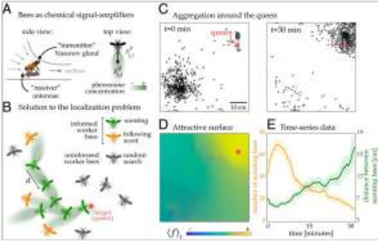




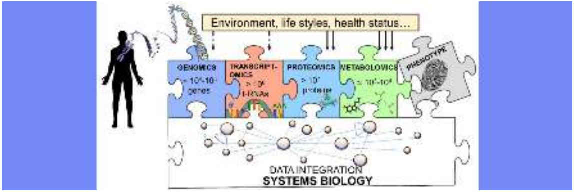


- Gene networks, functional brain networks, swarming behavior...

Relational networks: networks in biology

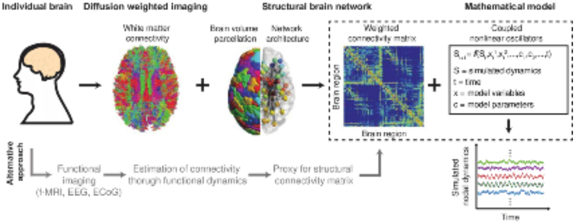
Examples

- Biochemical networks: metabolic, protein or gene interactions



are studied as deterministic models or Bayesian networks.

- Brain networks



- From ecology: herding, swarm intelligence, predator pray

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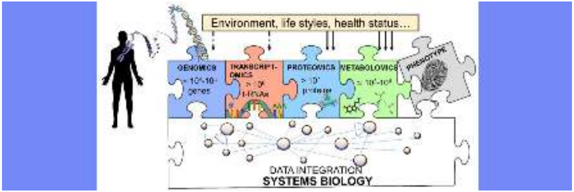

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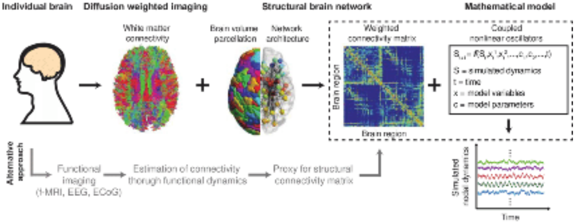

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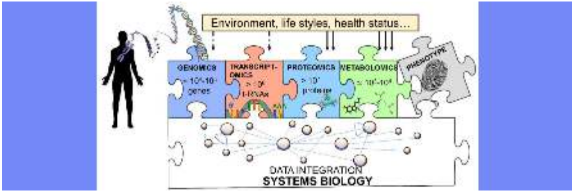

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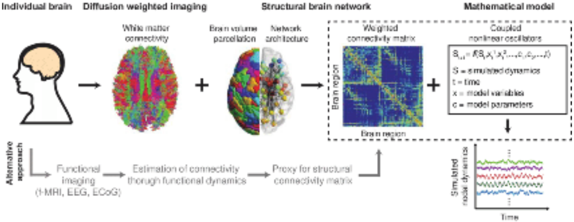

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Outline

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5 Examples of complex networks
- Relational networks
- Networks for data models
- Infrastructures

Data modeling networks

There two main classes of networks used to model data structures:

1. A class model for the **geometry** of deterministic data (a proxy for a *data manifold*)
   - Numerical data can be seen as points $\boldsymbol{x}_i \in \mathbb{R}^d$ (e.g. the pixels of an image). Geometric graphs can be used to represent their natural embedding in a lower dimensional surface.
   - We may want to map $\boldsymbol{x}_i$ onto a simpler object. Like a picture of a person onto a stick figure.

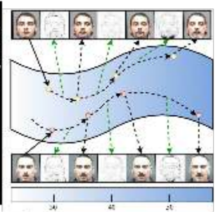
Outline

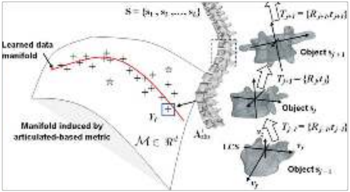
Cornell University

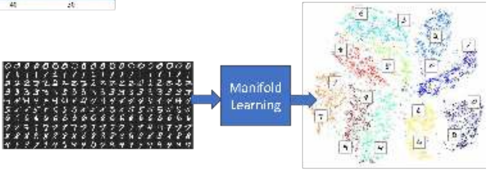
5 Examples of complex networks
- Relational networks
- Networks for data models
  - Data topology and Geometry
- Infrastructures

Data topology

- Geometric graphs formed with data $x_i \in \mathbb{R}^D$ $d > 1$ are proxies for manifolds of dimension $D' < D$ containing the data.
- Meshes are graph representations of complex objects (e.g. faces).







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Infrastructures

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These networks can be broadly classified in two types:

- Digital communication networks (supporting the data flow in the Internet) and transportation networks are modeled by flows of units from a source to a target.
  - The issue is *stability*. There is no force, but there is a limit in the amount of units that can flow and occupy the system.
- Electrical grids and gas pipelines are characterized by forces (Voltage = potential energy per unit of charge, Pressure = force per unit area) generating a current or gas to flow in the direction of lower voltage or pressure respectively.

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The Internet
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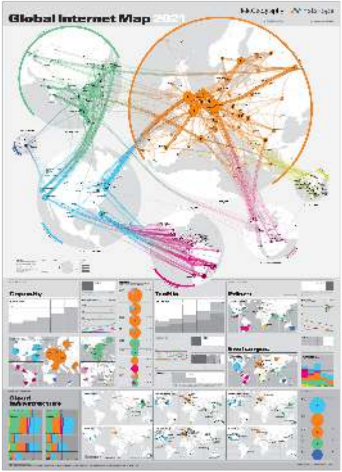

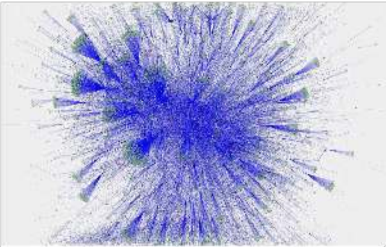

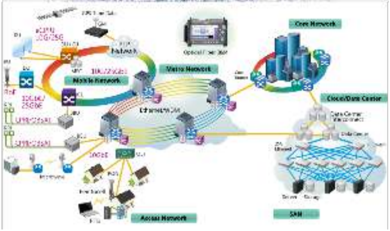

The Internet

Examples

- It is the set of physical connections that support the flow of packets from source to destinations, identified by an IP address
- Intermediate nodes are routers. Channels are duplex (allow for a bidirectional flow, i.e. is a multi-graph).
- Each link has a different capacity $c_{uv}[\text{Bytes} \times \text{sec.}]$ and the flow of data $0 \leq f_{uv}(t) \leq \overline{f}_{uv}$. Each node has a buffer storing queue of packets, whose state $q_i(t)$ is:

$$q_v(t) = q_v(t-1) + \sum_{u \in \mathcal{N}_v^+} f_{uv}(t) - \sum_{u \in \mathcal{N}_v^-} f_{vu}(t)$$

- Each flow is the sum of the traffic flows from each source-destination pair that is connected through that route.

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Internet nodes and edges fall into different classes:

- the backbone of high-bandwidth long-distance connections;
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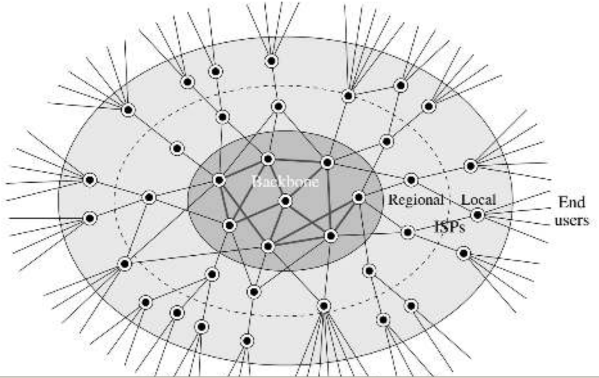

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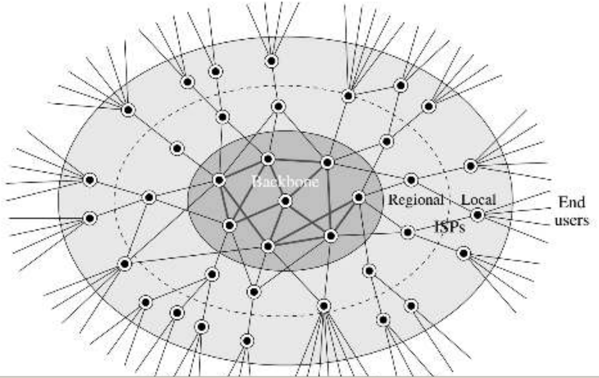

Transportation networks

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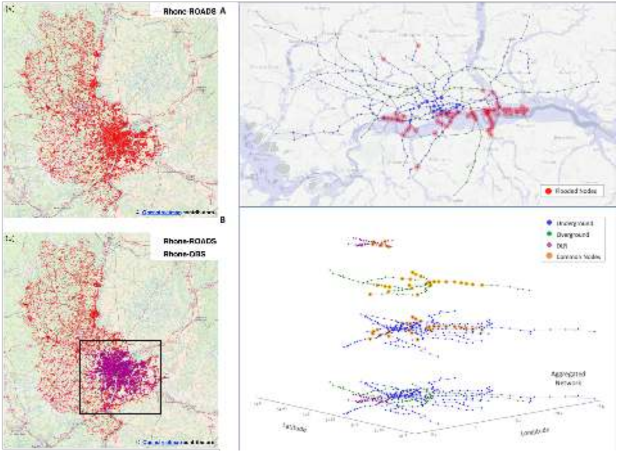

- Car, air, train coupled to support mobility of people and goods

Transportation networks

Examples

Cornell University

- The basic equations of transportation and communication networks flows are very similar: a source sends an item to a destination. Overall there is a balance of flows in and out of the road network.
- The delay is the typical metric for the cost of the route taken and in both cases is affected by the overall traffic.
- Among the difference is that the design of transportation networks is constrained by topography (more so than the Internet). Also, the travel speed is not predictable necessarily given the route. Only for wireless access that is true.

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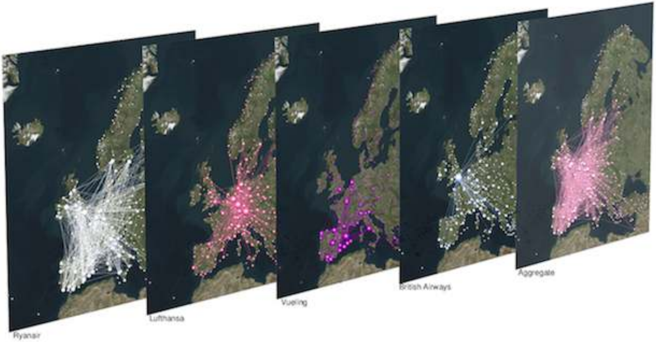
Transportation networks as multigraphs

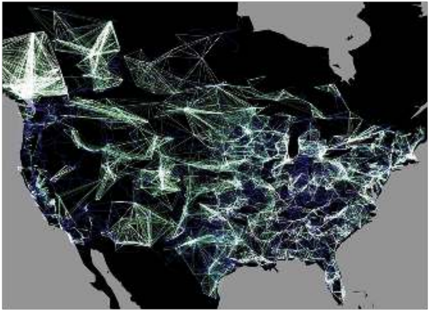
Examples

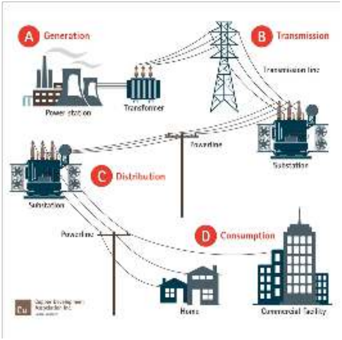
- If one considers the multiple ways of going from an origin to a destination, then the transportation network is a Multiplex network, which mathematically is a multigraph



The electric grid

Examples





- The transmission grid is high-voltage and meshed. The distribution grids are (mostly) radial and include medium voltage and a low voltage sections, that connect to the customer premises.

The electric grid

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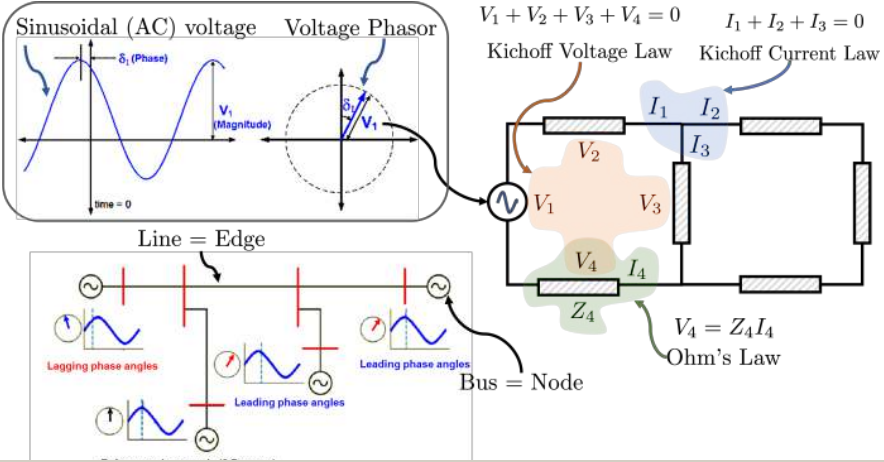
- Kirchoff's voltage and current laws and Ohm's law govern the transmission of power. They are a simplification of Maxwell's Electromagnetic Fields equations.



The electric grid

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- The transmission lines interconnections form the network topology.
  - The nodes (called *buses*), are a classified in *load*, *generation* buses (they can be both) or intermediate buses.
    - Generation buses *inject* positive power and loads *inject* negative power.
  - The edges (called *lines*) are weighted by the admittance of the line y_{uv} (the reciprocal of the resistance).
  - In terms of phasors, power in a line $S^*_{uv} = (V_i - V_j)I^*$, and at a node is $S_i = V_i I_i^*$. Maximum power transfer is when S_i is real.

More details will follow in the modeling part...

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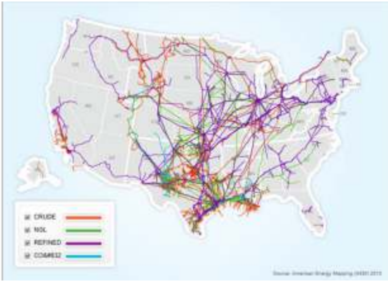
Pipelines
Examples



- The flow of gas (compressible) and water/oil (incompressible) in a pipe are special cases of Navier-Stockes equations. They often simplified into one-dimensional isothermal Euler equations that ignore viscosity.

Gas Pipelines (Node types)

Examples

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Node Type	Description	Facilities
demand ($L > 0$)	point, where gas is extracted from the network, connected facilities are typically flow or pressure controlled	CGS, CBE, GFPP, IND
supply ($L < 0$)	point, where gas is injected into the network; connected facilities are typically flow or pressure controlled; for LNG regasification terminals the working gas inventory is monitored and the flow rate is reduced in case of low inventory	PRO, CBI, LNG
storage ($L \geq 0$ or $L \leq 0$)	point, where gas is injected or extracted from the network and where the maximum supply/loads depend on the working gas inventory, which is monitored along the transient simulation; connected facilities are typically flow or pressure controlled	UGS
junction ($L = 0$)	point, where a topological change or a change in pipe properties occurs (e.g., diameter, inclination); no specific control	-

Different connections.[2]

[2] Facilities: compressor stations (CS), production fields (PRO), cross-border import (CBI) and export stations (CBE), city gate stations (CGS), stations of direct served customers (GFPPs, IND), liquefied natural gas (LNG) regasification terminals and underground gas storage (UGS).

Gas Pipelines (Elements/Lines)

Examples

Element Types	Description
Passive Elements	
pipe	models a section of a pipeline, basic properties are length, diameter, roughness and pipe efficiency
resistor	models passive devices that cause a local pressure drop (e.g., meters, inlet piping, coolers, heaters, scrubbers etc.)
Active Elements	
compressor	models a compressor station with generic constraints, allows the specification of a control mode of the station (e.g., outlet pressure control, inlet pressure control, flow rate control etc.)
regulator	models a pressure reduction and metering station located at the interface of two neighboring networks with different maximum operating pressures, allows the specification of a control mode of the station (e.g., outlet pressure control, inlet pressure control, flow rate control etc.)
valve	models a valve station, which is is either opened or closed

Different elements.

Outline

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Conclusions

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- The modeling of various processes and data through networks allows to apply specialized knowledge for algorithms and feature extraction.
- The first step is mapping the network onto the appropriate graph and specific graph attributes.
- To start with processing the data, we need to know basic graph theory concepts, which are the unifying thread between all these different data sources.
- Next time we will further our understanding of graph theory and graph data analysis.

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