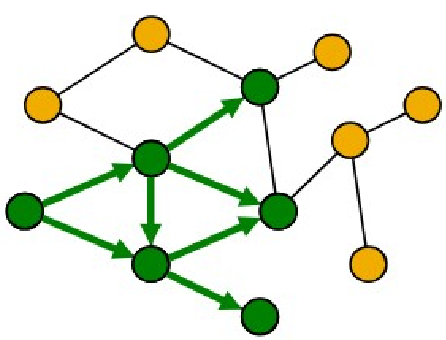
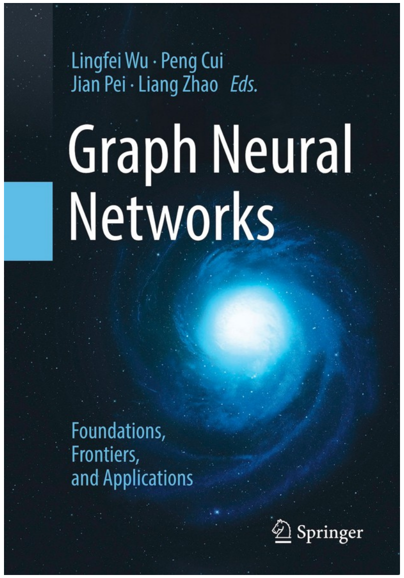
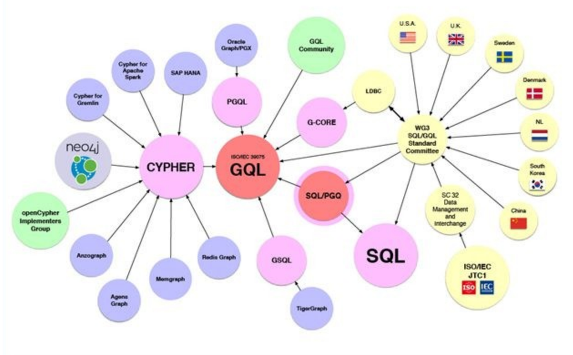
Other Topics
(wrapping up the NetSci course)

Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)



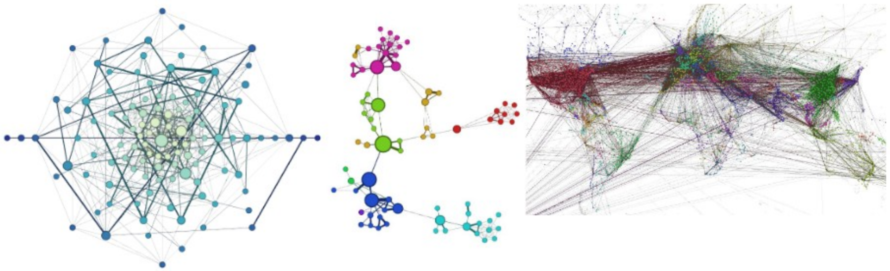




Remembering Our Classes

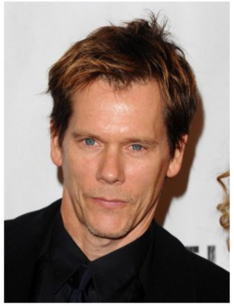
An Introduction To Network Science

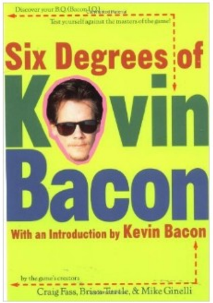
Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)



More examples of "Small World"

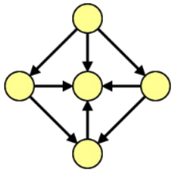
- The six degrees of Kevin Bacon
  - How many connections to link Kevin Bacon to any other actor, director, producer...
  - "Game" initiated in 1994

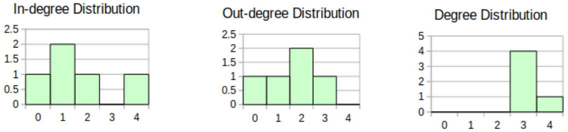




Node Properties

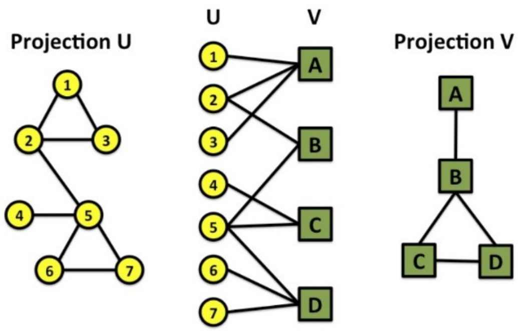
- **Degree related metrics:**
  - **Degree sequence**
    an ordered list of the (in,out) degree of each node
    - In-degree sequence: [4, 2, 1 , 1, 0]
    - Out-degree sequence: [3, 2, 2, 1, 0]
    - Degree sequence: [4, 3, 3, 3, 3]
  - **Degree Distribution**
    a frequency count of the occurrences of each degree
    [usually plotted as probability → normalization]





Bipartite

- **A bipartite graph is a graph whose nodes can be divided into two disjoint sets U and V such that every edge connects a node in U to one in V.**



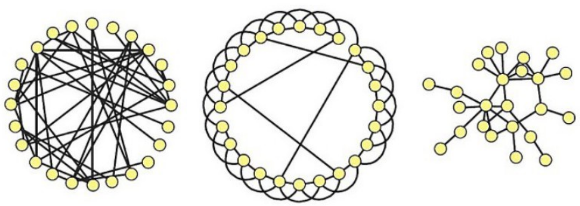
Example:
- Actor Network
  . U = Actor
  . V = Movies

Image: Adapted from Leskovec, 2015

2 - Measuring Networks and Random Graph Models

Measuring Networks and Random Graph Models

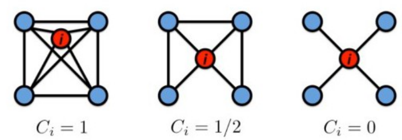
Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)



(Heavily based on slides from Jure Leskovec and Lada Adamic@ Stanford University - CS224W)

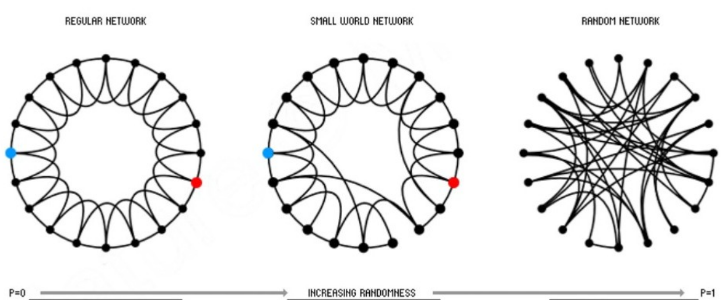
(3) Clustering Coefficient

- **Clustering coefficient**:
  - What portion of ***i***'s neighbors are connected?
  - Node ***i*** with degree $\boldsymbol{k_i}$
  - $C_i \in [0,1]$
  - $C_i = \frac{2 e_i}{k_i(k_i - 1)}$ where e_i is the number of edges between the neighbors of node i



- **Average clustering coefficient:** $C = \frac{1}{N} \sum_{i}^{n} C_i$

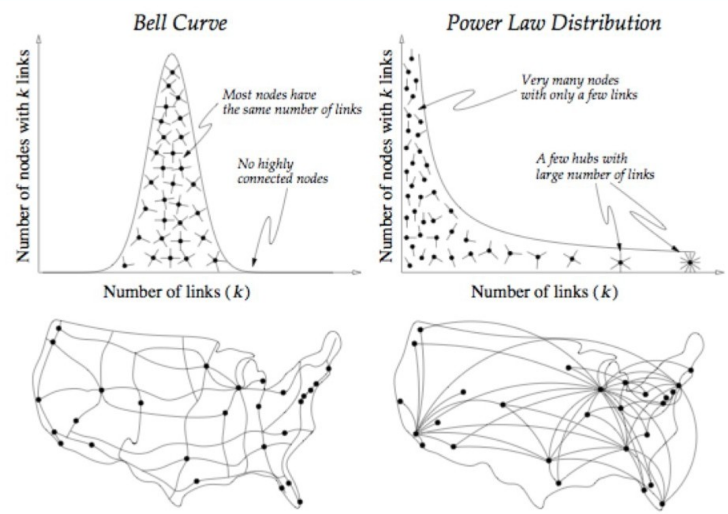
The Small World Model



High clustering High diameter	High clustering Low diameter	Low clustering Low diameter
$h = \frac{N}{2\bar{k}}$ $C = \frac{1}{2}$		$h = \frac{\log N}{\log \alpha}$ $C = \frac{\bar{k}}{N}$

Rewiring allows us to "interpolate" between a regular lattice and a random graph

Interpreting Power-Laws



3 – Node Centrality

Node Centrality

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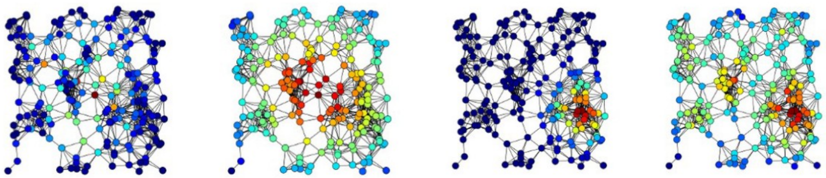
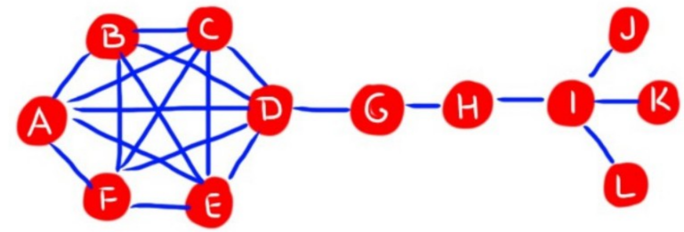
(DCC/FCUP & CRACS/INESC-TEC)



(Heavily based on slides from Jure Leskovec and Lada Adamic @ Stanford University)

Betweenness: Question

- Find a node that has **high betweenness** but **low degree**



Closeness: Definition

- **Closeness** is based on the **length of the average shortest path** between a node and all other nodes in the network

Closeness Centrality:

$$C_C(i) = \frac{1}{\sum_{j=1}^{N} d(i,j)}$$

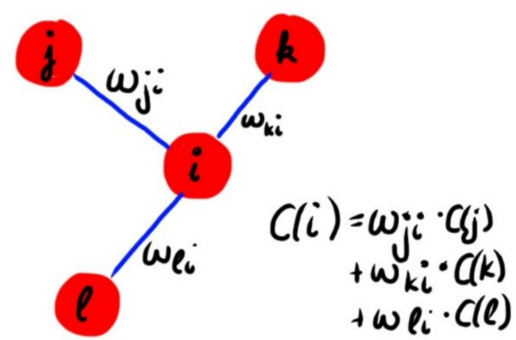
Normalized Closeness Centrality:

$$C'_C(i) = C_C(i) \times (n-1)$$

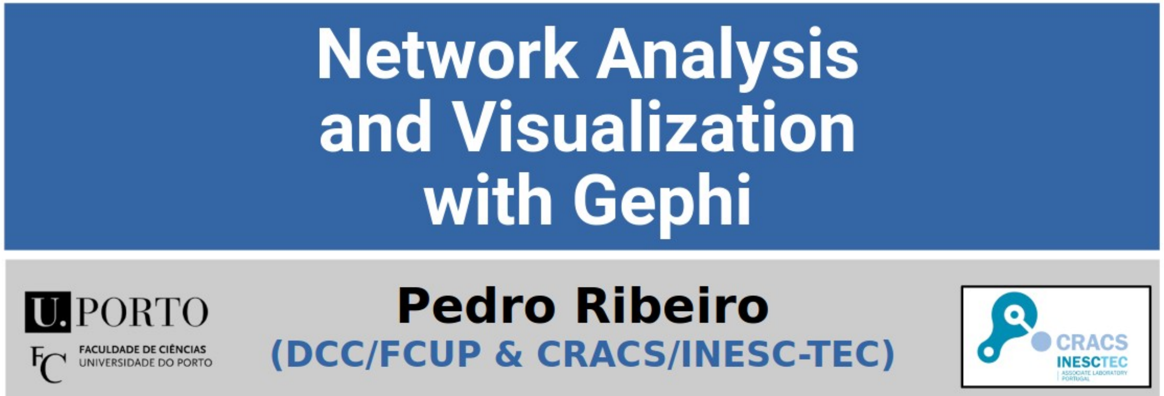
When graphs are big, the -1 can be discarded and we multiply by *n*

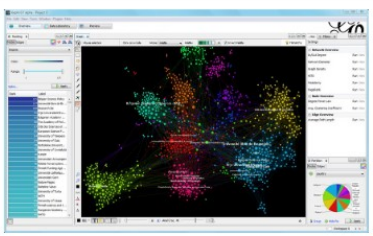
Eigenvector Centrality

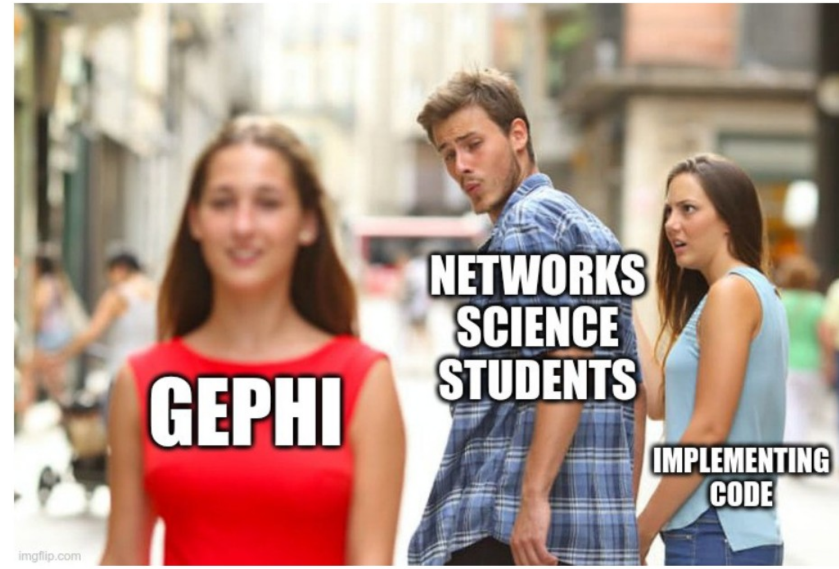
- How "central" you are depends on how "central" your neighbors are

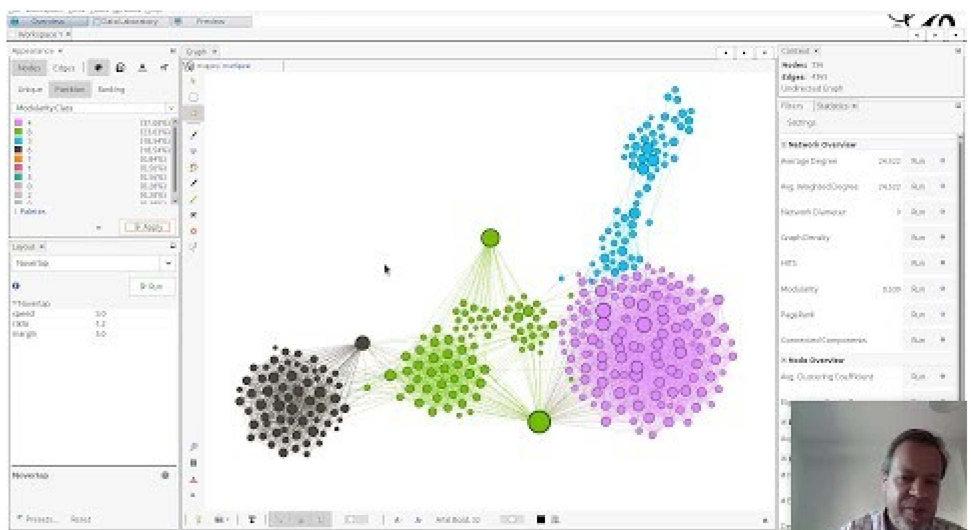


4 - Network Analysis and Visualization with Gephi









5 – Link Analysis

Link Analysis: PageRank

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Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)

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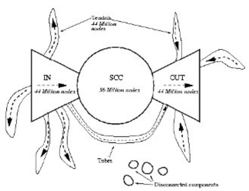
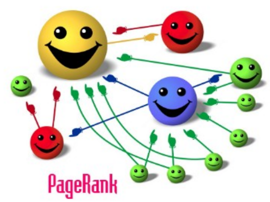




(Heavily based on slides from Jure Leskovec and Lada Adamic @ Stanford University)

Structure of the Web

- **Broder et al.**: Altavista web crawl (Oct '99)
  - Web crawl is based on a large set of starting points accumulated over time from various sources, including voluntary submissions.
  - 203 million URLS and 1.5 billion links

Goal: Take a large snapshot of the Web and try to understand how its SCCs "fit together" as a DAG

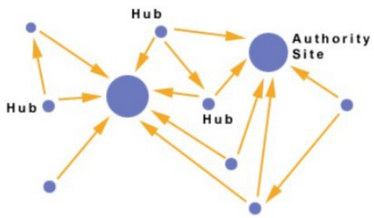
Tomkins, Broder, and Kumar

Hubs and Authorities

Interesting pages fall into two classes:

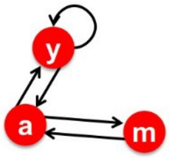
1) Authorities are pages containing useful information
- Newspaper home pages
- Course home pages
- Home pages of auto manufacturers

2) Hubs are pages that link to authorities
- List of newspapers
- Course bulletin
- List of auto manufacturers



PageRank: How to Solve?

- **Power Iteration:**
  - Set $r_j \leftarrow 1/N$
  - **1:** $r'_j \leftarrow \sum_{i \to j} \frac{r_i}{d_i}$
  - **2:** $r \leftarrow r'$
  - If $|r - r'| > \varepsilon$: goto **1**
- **Example:**



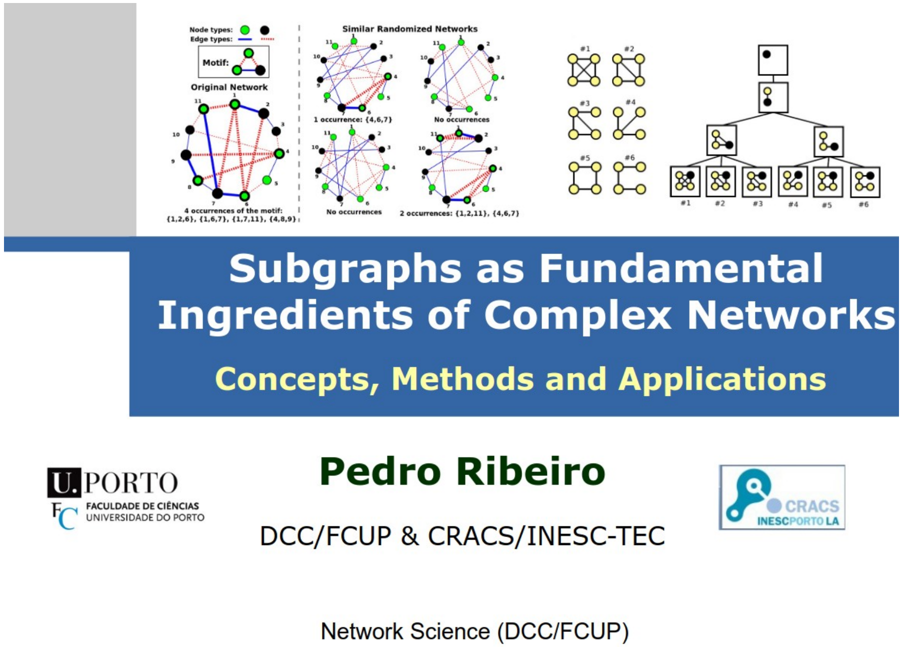
	y	a	m
y	½	½	0
a	½	0	1
m	0	½	0

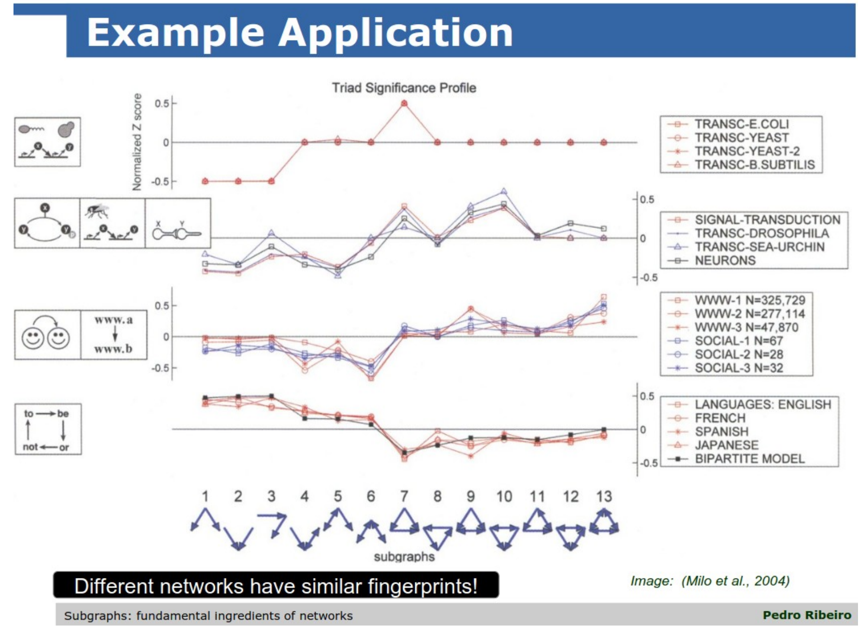
$r_y = r_y/2 + r_a/2$
$r_a = r_y/2 + r_m$
$r_m = r_a/2$

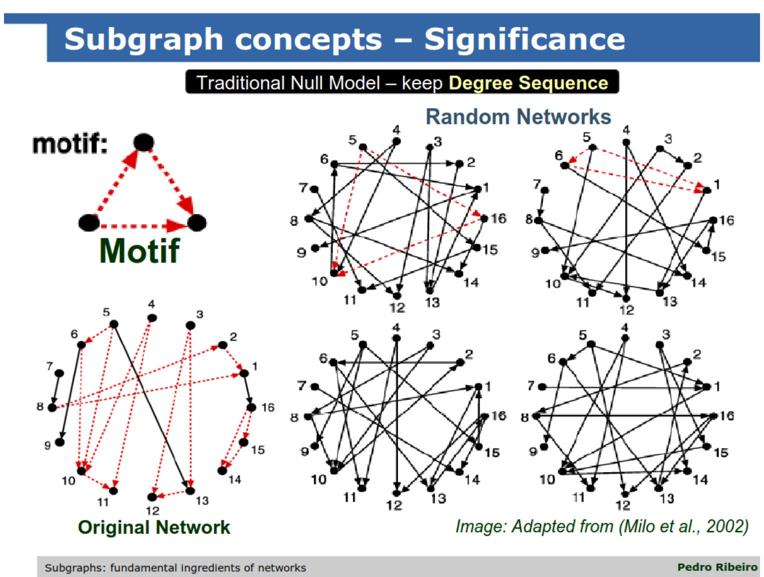
$$\begin{bmatrix} r_y \\ r_a \\ r_m \end{bmatrix} = \begin{matrix} 1/3 & 1/3 & 5/12 & 9/24 & & 6/15 \\ 1/3 & 3/6 & 1/3 & 11/24 & \ldots & 6/15 \\ 1/3 & 1/6 & 3/12 & 1/6 & & 3/15 \end{matrix}$$

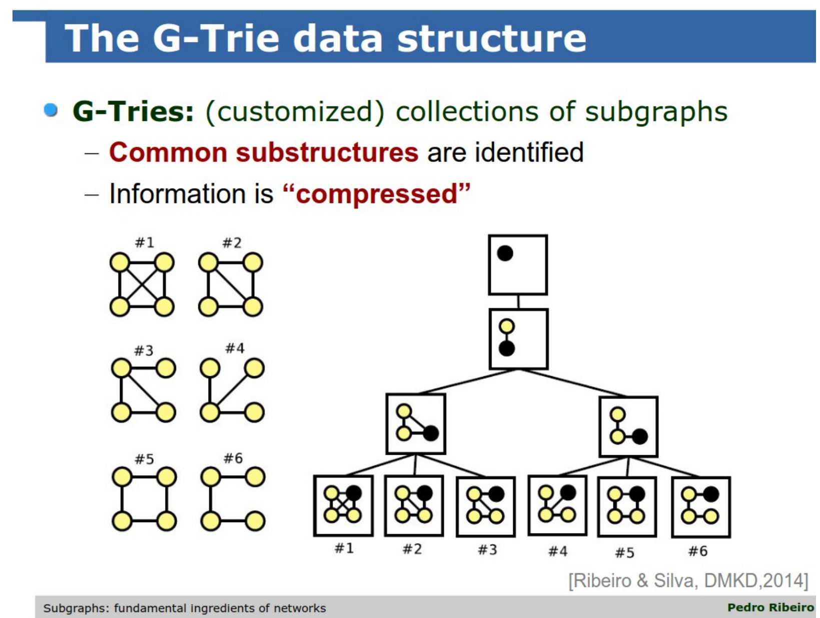
Iteration 0, 1, 2, …

6 - Subgraph Patterns





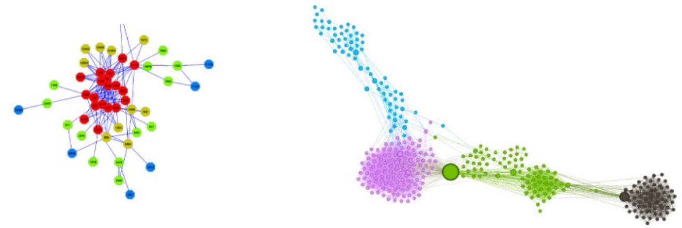




7 - Roles and Community Structure

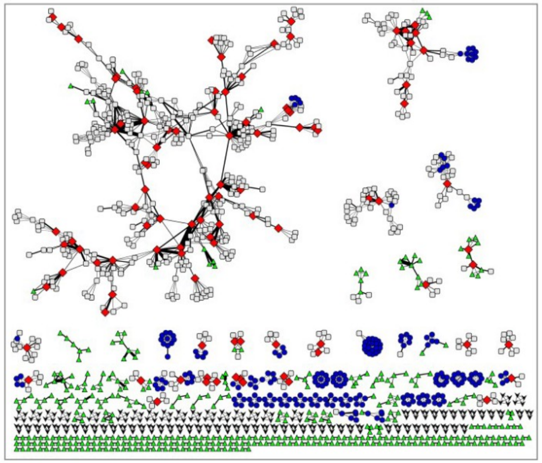
Community Structure in Networks

Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)



(Mainly selected slides from Jure Leskovec and Gonzalo Mateos)

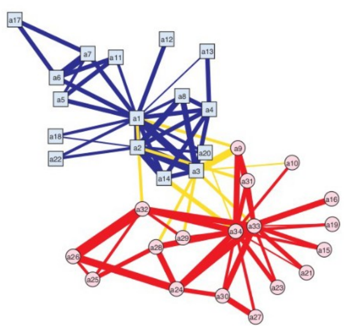
Examples of Roles



Network Science Co-authorship network [Newman 2006]

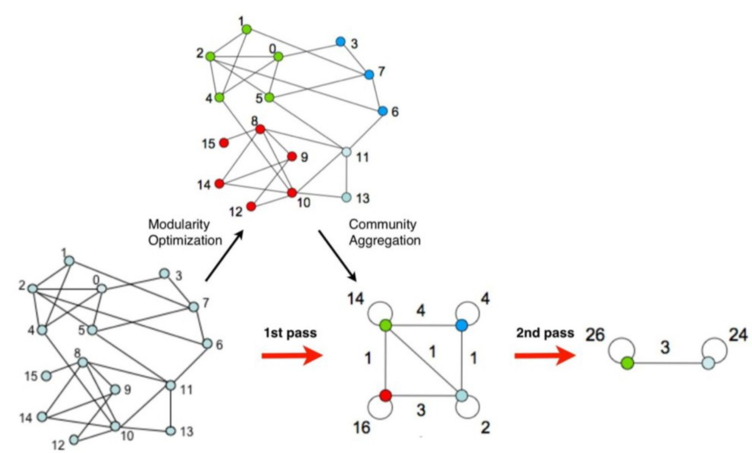
Zachary's karate club

- Social interactions among members of a karate club in the 70s



- Zachary witnessed the club split in two during his study
  - ⇒ Toy network, yet canonical for community detection algorithms
  - ⇒ Offers "ground truth" community membership (a rare luxury)

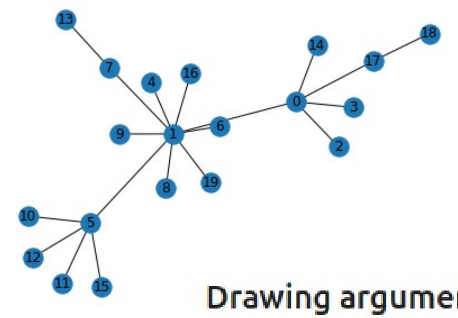
Louvain Algorithm Overview



8 - Analyzing networks with NetworkX

NetworkX
Network Analysis in Python

```
# Returns a random Barabasi-Albert graph with n=20 nodes and each new node connects to m=1 nodes
G = nx.barabasi_albert_graph(20,1)
nx.draw(G, with_labels=True)
```

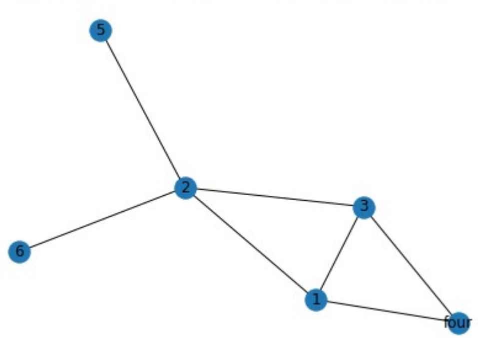


Adding edges and nodes explicitly

Here is our first example of an undirected graph:

```
# Create an empty undirected graph
G = nx.Graph()

# Create some nodes
G.add_node(1)              # create a single node
G.add_nodes_from([2,3])    # create nodes from a list
G.add_node("four")         # node labels can be of different types (anything hashable)

# Create some edges
G.add_edge(1,2)
G.add_edges_from([(2,3),(3,"four"), ("four", 1), (1,3)])
G.add_edges_from([(2,5),(2,6)]) # if a node does not exist, it is created

# Show nodes and edges
print(G.nodes)
print(G.edges)

# Draw the graph (more on this later)
nx.draw(G, with_labels = True)
```

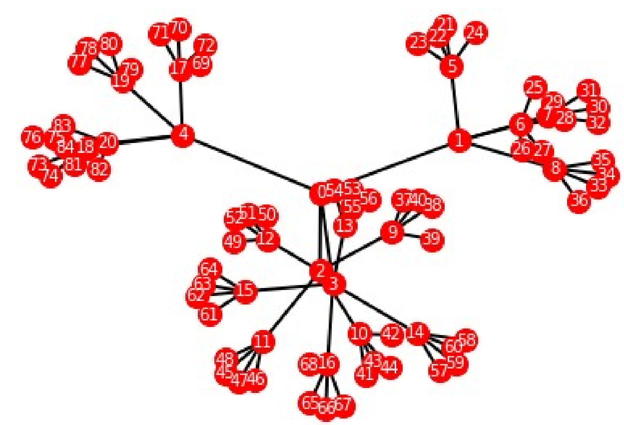
```
[1, 2, 3, 'four', 5, 6]
[(1, 2), (1, 'four'), (1, 3), (2, 3), (2, 5), (2, 6), (3, 'four')]
```



Drawing arguments

It accepts many possible arguments:

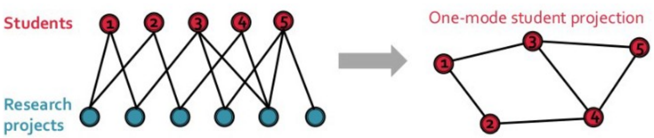
```
G = nx.balanced_tree(4,3)

nx.draw(G, with_labels=True,
        node_size=200,      # size of nodes
        font_size=10,       # text label size
        node_color="red",   # color of nodes
        font_color="white", # color of nodes
        width=2,            # width of edges
        pos=nx.spring_layout(G, iterations=500, k=1.5)
        )
```

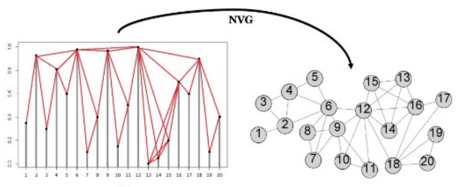


9 - Network Construction

Network Construction

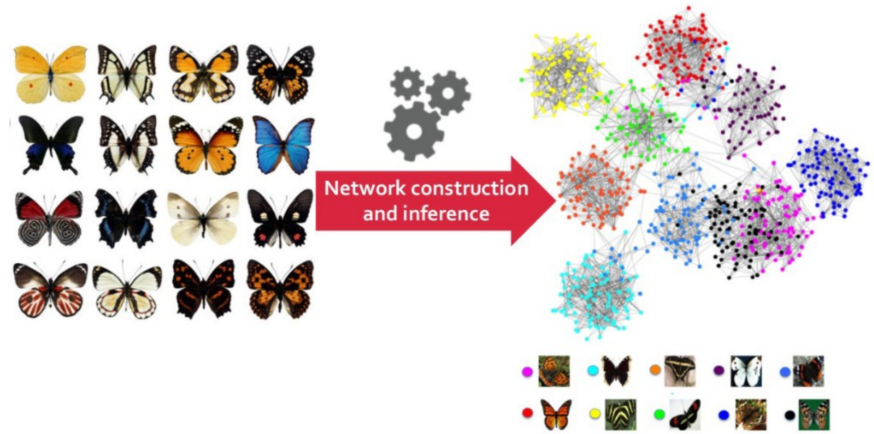
Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)





(Mainly selected slides from Jure Leskovec, Lucas Lacasa and Vanessa Silva)

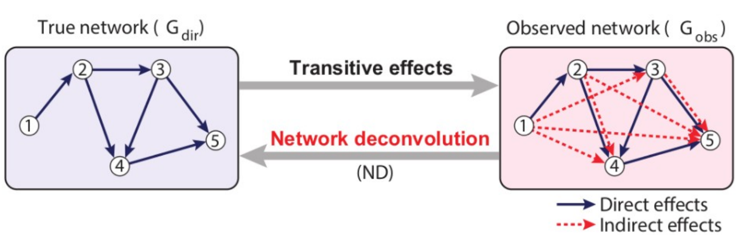
How to construct networks?



Today: How to construct and infer networks from raw data?

Network Deconvolution

- **Goal:** Reverse the effect of transitive information flow across all indirect paths:
  - Recover **true direct network (blue edges, G_{dir})** based on **observed network (combined blue and red edges, G_{obs})**

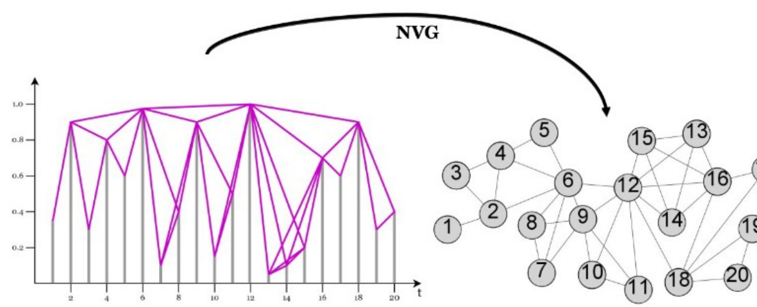


Feizi *et al.*, *Nature Biotechnology*, 31:8, 2013.

Visibility Graphs

$$y_c = y_b + (y_a - y_b)\frac{(t_b - t_c)}{t_b - t_a}, \qquad t_a < t_c < t_b$$

Natural Visibility Graph



10 - Link Prediction

Link Prediction: an introduction

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Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)

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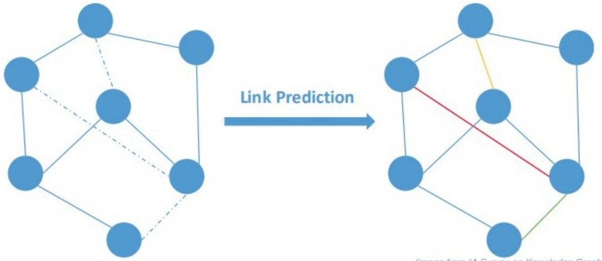


(image from "A Survey on Knowledge Graph Embeddings for Link Prediction")

(based on slides used by myself at PBS and by Marcia Oliveira)

Link Prediction: Methods

A Survey of Link Prediction in Complex Networks

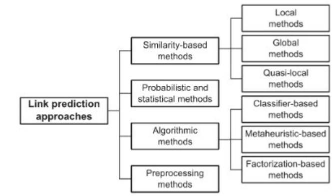
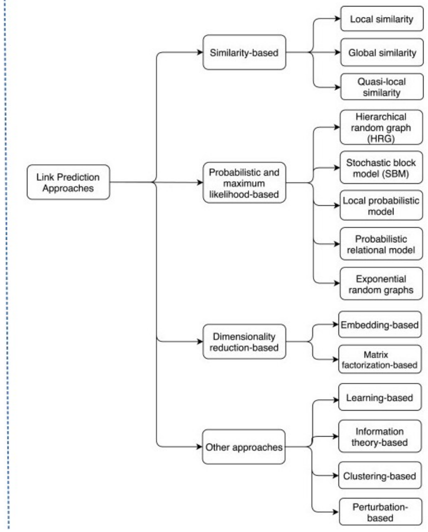


Fig. 1. Our proposed taxonomy for link prediction techniques.



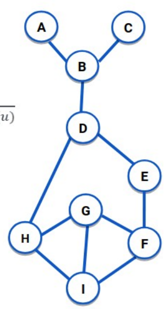
Resource Allocation Index

- Fraction of a "resource" that a node can send to another through their common neighbors

How to compute?

$$res\_alloc(i, j) = \sum_{u \in N(i) \cap N(j)} \frac{1}{|N(u)|} = \sum_{u \in N(i) \cap N(j)} \frac{1}{degree(u)}$$

N(i)/N(j) – set of neighbors of node i/ node j



Example:

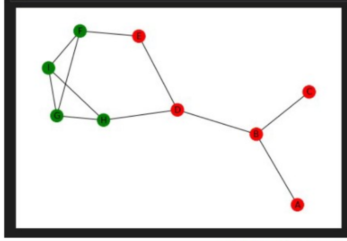
$$res\_alloc(F, H) = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}$$

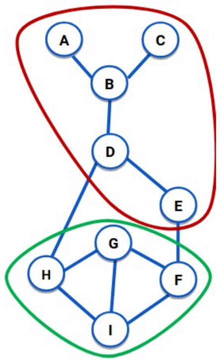
Community-based measures

Community-based measures

```python
G.nodes['A']['community'] = 0
G.nodes['B']['community'] = 0
G.nodes['C']['community'] = 0
G.nodes['D']['community'] = 0
G.nodes['E']['community'] = 0

G.nodes['F']['community'] = 1
G.nodes['G']['community'] = 1
G.nodes['H']['community'] = 1
G.nodes['I']['community'] = 1

colors = { 0 : 'red', 1 : 'green'}
communities = [colors[G.nodes[node]['community']] for node in G.nodes()]

nx.draw(G, with_labels=True, node_color=communities)
```

✓ 0.9s Python

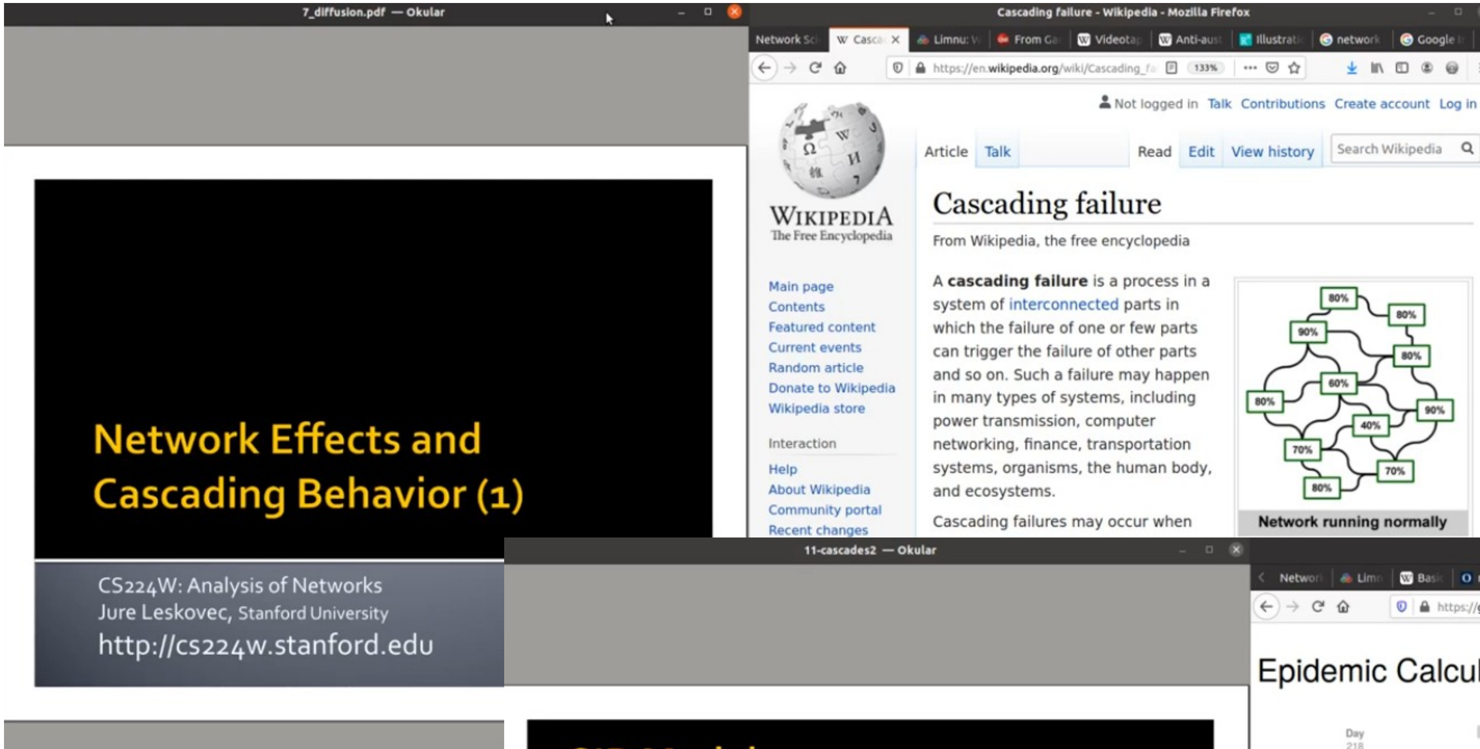


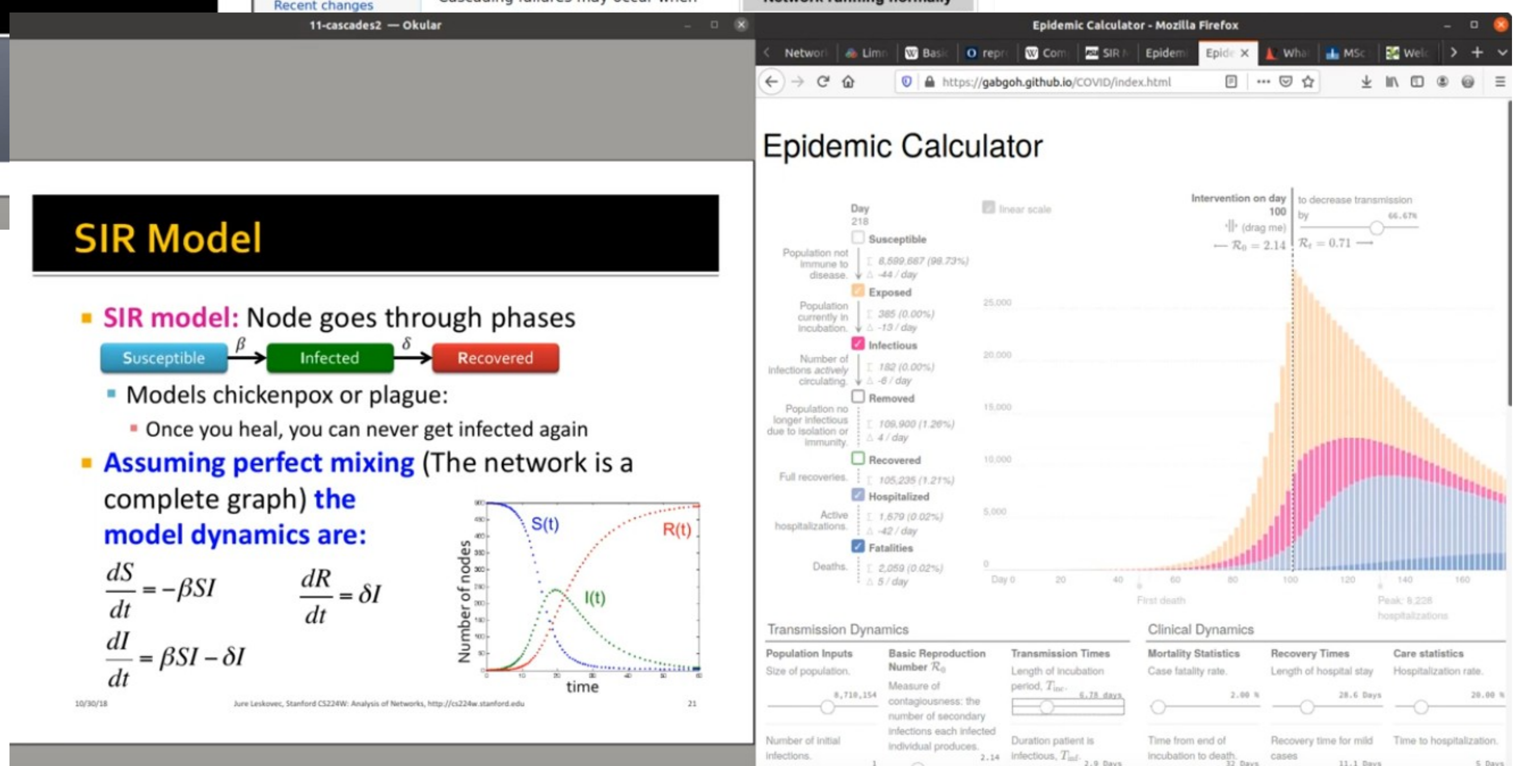


NetworkX Network Analysis in Python

Other Material

Diffusion and Cascading Behavior



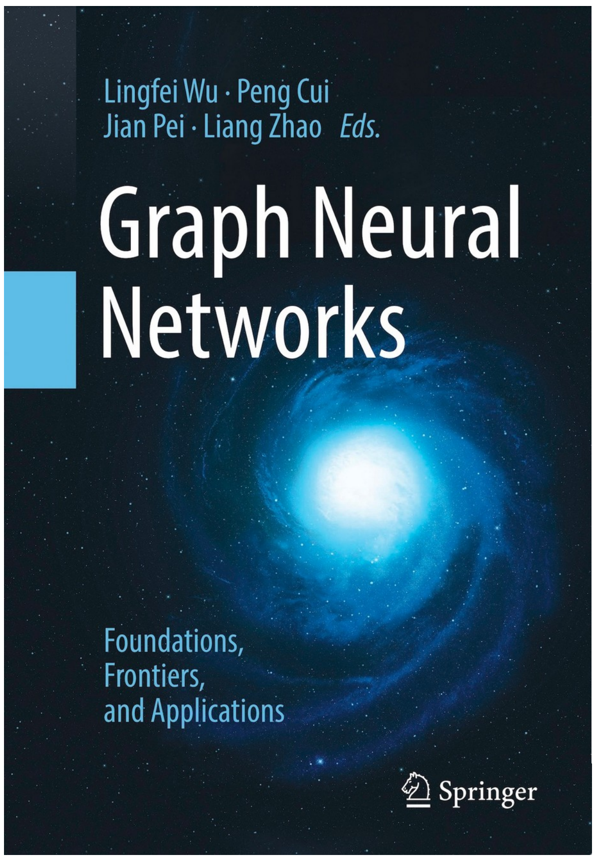


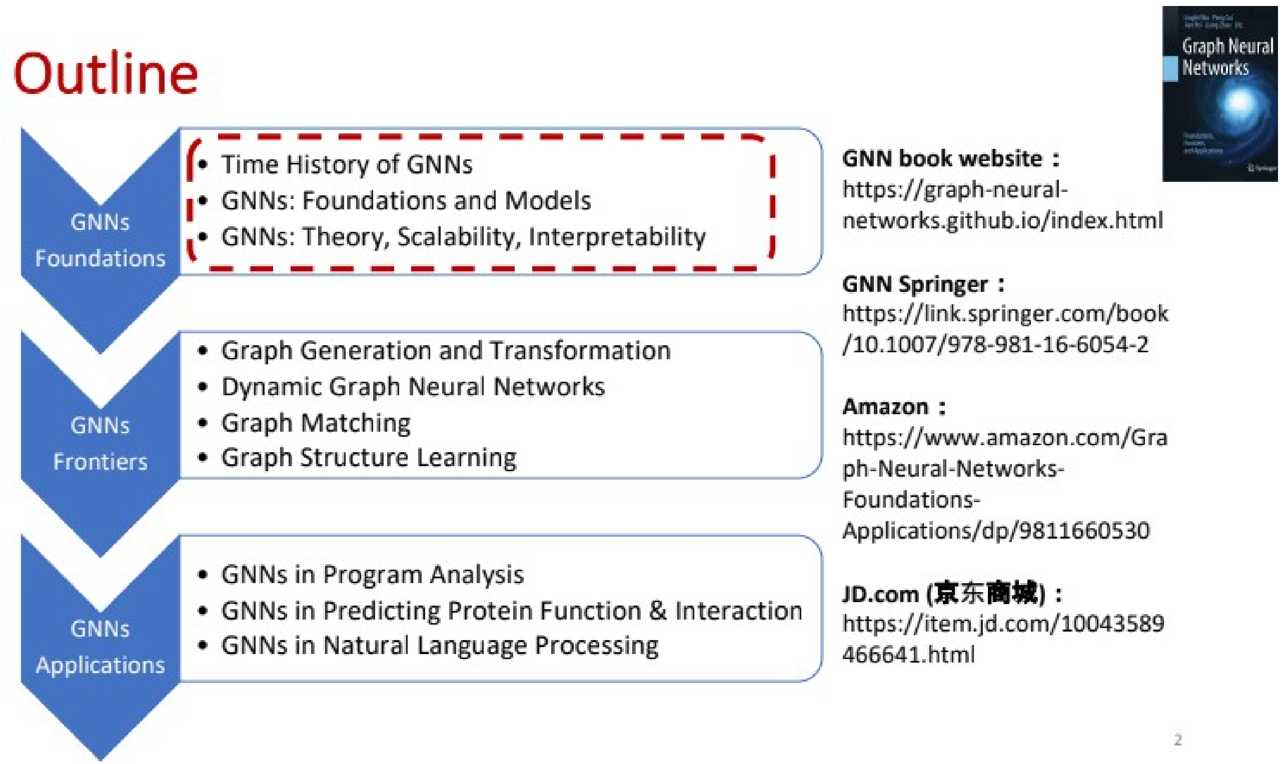
Slides and Videos
from previous courses
are available
on the website

Graph Neural Networks

- *“deep learning meets network science”*

https://graph-neural-networks.github.io/





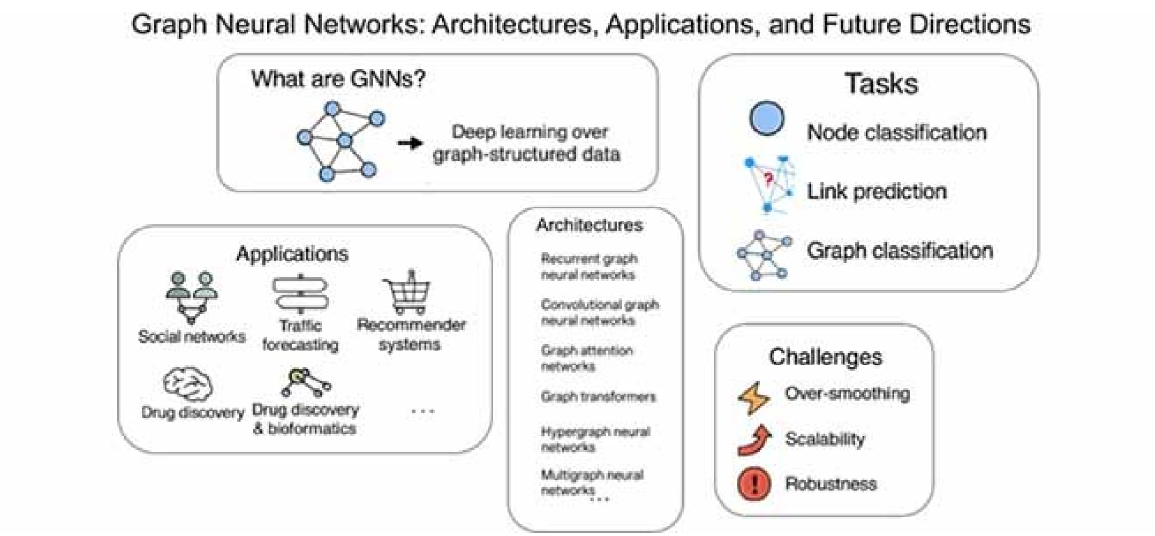
PyG

DGL DEEP GRAPH LIBRARY

GNNs Literature

Graph Neural Networks: Architectures, Applications, and Future Directions

VALERIO PONZI[1,2] AND CHRISTIAN NAPOLI[1,2,3]
[1]Department of Computer, Control, and Management Engineering, Sapienza University of Rome, 00185 Rome, Italy
[2]Institute for Systems Analysis and Computer Science, Italian National Research Council, 00185 Rome, Italy
[3]Department of Mathematics Applications and Methods for Artificial Intelligence, Silesian University of Technology, 44-100 Gliwice, Pol
Corresponding author: Valerio Ponzi (ponzi@diag.uniroma1.it)



Primer

Check for updates

Graph neural networks

Gabriele Corso[1,3], Hannes Stark[1,3], Stefanie Jegelka[1,2], Tommi Jaakkola[1] & Regina Barzilay[1]

Abstract

Graphs are flexible mathematical objects that can represent many entities and knowledge from different domains, including in the life sciences. Graph neural networks (GNNs) are mathematical models that can learn functions over graphs and are a leading approach for building predictive models on graph-structured data. This combination has enabled GNNs to advance the state of the art in many disciplines, from discovering new antibiotics and identifying drug-repurposing candidates to modelling physical systems and generating new molecules. This Primer provides a practical and accessible introduction to GNNs, describing their properties and applications to the life and physical sciences. Emphasis is placed on the practical implications of key theoretical limitations, new ideas to solve these challenges and important considerations when using GNNs on a new task.

Sections

CASE STUDY **Open Access**

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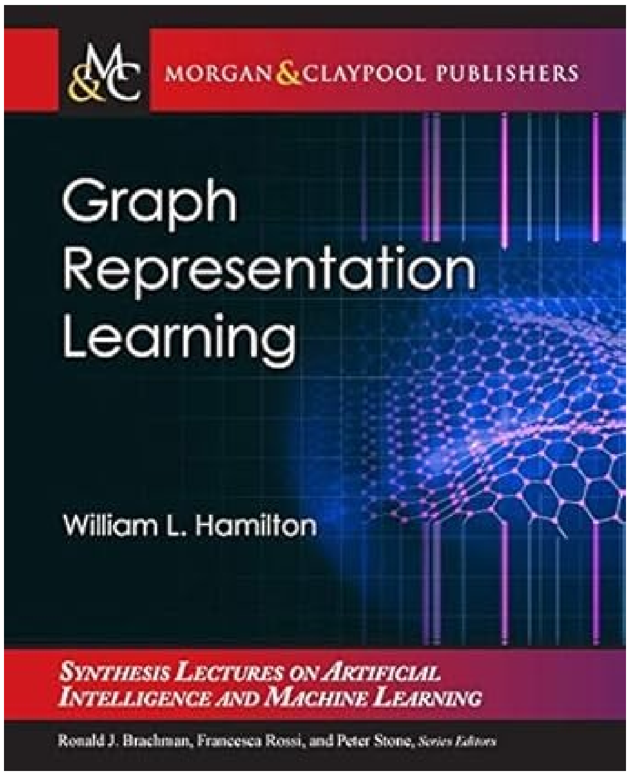
A review of graph neural networks: concepts, architectures, techniques, challenges, datasets, applications, and future directions

A Survey on Graph Neural Networks and its Applications in Various Domains

Graph Representation Learning

https://www.cs.mcgill.ca/~wlh/grl_book/



Machine Learning With Graphs

https://web.stanford.edu/class/cs224w/

CS224W: Machine Learning with Graphs

Stanford / Fall 2024

Logistics

- **Lectures:** are on Tuesday/Thursday 3:00-4:20pm **in person** in the NVIDIA Auditorium.
- **Lecture Videos:** are available on Canvas for all the enrolled Stanford students.
- **Public resources**: The lecture slides and assignments will be posted online as the course progresses. We are happy for anyone to use these resources, but we cannot grade the work of any students who are not officially enrolled in the class.
- **Contact**: Students should ask *all* course-related questions on Ed (accessible from Canvas), where you will also find announcements. For external inquiries, personal matters, or in emergencies, you can email us at *cs224w-aut2425-staff@lists.stanford.edu*.
- **Academic accommodations**: If you need an academic accommodation based on a disability, you should initiate the request with the Office of Accessible Education (OAE). The OAE will evaluate the request, recommend accommodations, and prepare a letter for the teaching staff. Once you receive the letter, send it to our staff email address. Students should contact the OAE as soon as possible since timely notice is needed to coordinate accommodations.

Instructor

Jure Leskovec

Course Assistants

Kexin Huang (Head CA)

Aman Patel

Harper Hua

1 

Stanford CS224W: Machine Learning with Graphs | 2021 | Lecture 1.1 - Why Graphs

Stanford Online • 522 mil visualizações • há 4 anos

2 

Stanford CS224W: Machine Learning with Graphs | 2021 | Lecture 1.2 - Applications of Graph ML

Stanford Online • 164 mil visualizações • há 4 anos

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Stanford CS224W: Machine Learning with Graphs | 2021 | Lecture 1.3 - Choice of Graph Representation

Stanford Online • 126 mil visualizações • há 4 anos

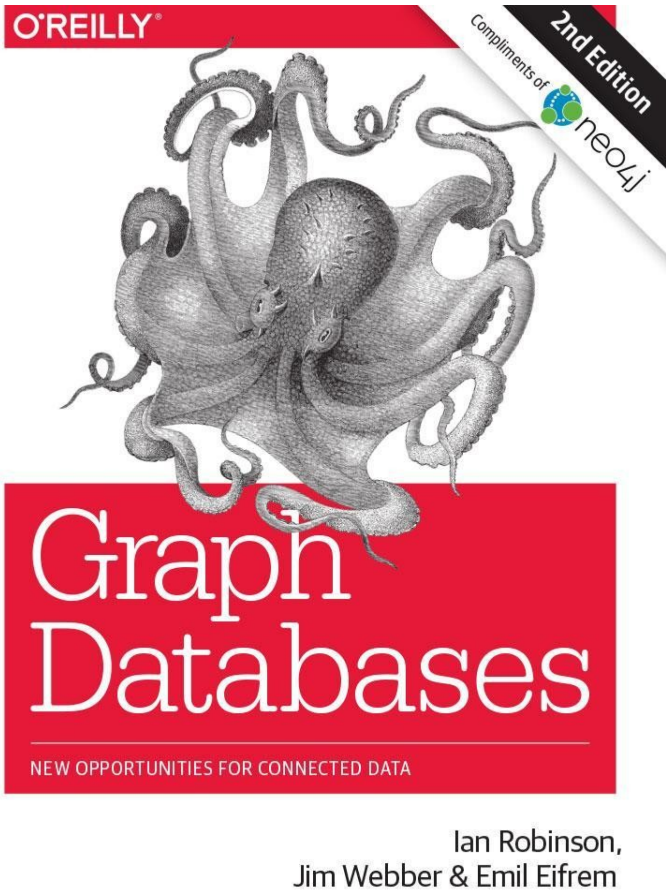
4 

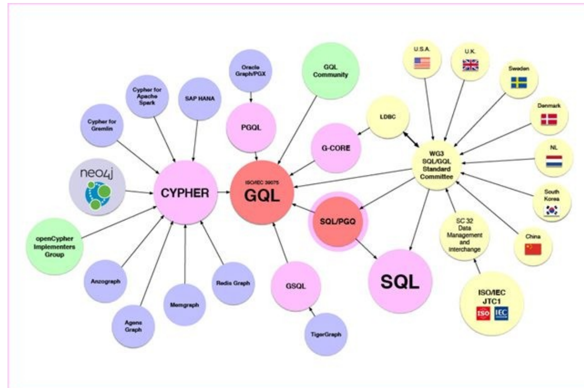
Stanford CS224W: ML with Graphs | 2021 | Lecture 2.1 - Traditional Feature-based Methods: Node

Stanford Online • 136 mil visualizações • há 4 anos

Graph Databases

https://en.wikipedia.org/wiki/Graph_database





MSc Thesis in/with Network Science

Examples of recent MSc Students

- [MCC] P. Daniel (25/26): **Algorithmic techniques for transforming temporal data into and from complex networks**
- [MCC] V. Abrunhosa (25/26): **Network Science Approaches to Political Dynamics**
- [MDS] M. Zhokhova (25/26): **Predicting disease-associated genes using graph approaches**
- [MDS] A. Chessa (25/26): **Detecting Fraud in Cryptocurrency Transactions Using Machine Learning and Graph-based Models**
- [MCC] P. Vieira (23/24): **Studying GNNs and their Capabilities for Finding Motifs**
- [MCC] D. Ferreira (23/24): **Football passing sequences and networks for goal prediction**
- [MBBC] D. Kumar (22/23): **Unravelling the Complexity of Human Disease: Transcriptomic Networks of Phenotype – Gene Expression Data**
- [MCC] J. Ferreira (21/22): **Subgraph Patterns in Spatial Networks**
- [MDS] F. Justiça (21/22): **Time series forecasting via Network Science**
- [MCC] M. Lamas (21/22): **Characterizing Music through Complex Networks**
- [MCC] I. Novo (21/22): **On the Summarization of Complex Networks**
- [MEAE] J. Trindade (21/22): **Spotting fraud: detecting patterns and red flags in financial networks**
- [MCC] B. Pinto (20/21): **Subgraph Patterns in Colored Networks**
- [MCC] H. Branquinho (19/20): **Counting Subgraphs in Streaming Networks**
- [MCC] F. Bento (19/20): **Characterizing the Passing Networks of Football Teams**
- [MCC] L. Grácio (18/19): **From Supergraph Counting to Subgraph Generation**
- [MERSI] A. Meira (18/19): **Subgraph Patterns in Multiplex Networks**
- [MCC] M. Martins (18/19): **Condensed Graphs: Towards a General Approach for Faster Subgraph Census**
- [MCC] A. Cascais (17/18): **Adaptive Parallel Subgraph Sampling in Large Complex Networks**

Me, Myself... and Graphs!