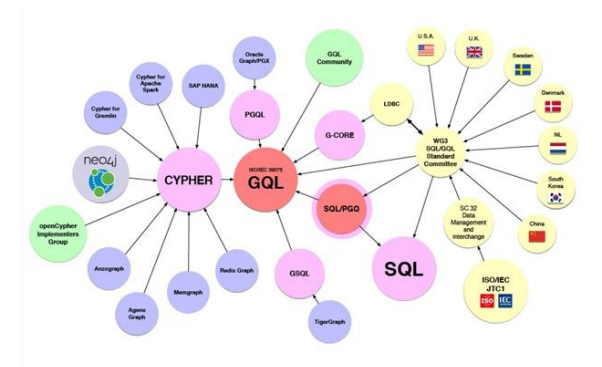
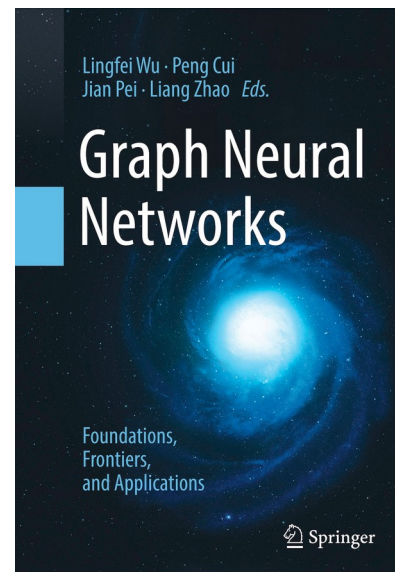
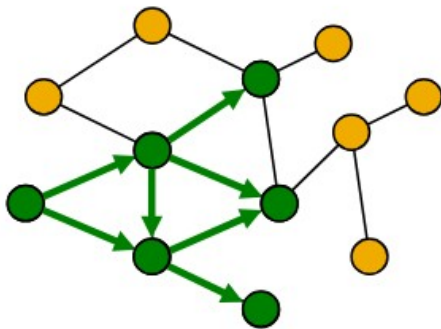


Other Topics (wrapping up the NetSci course)



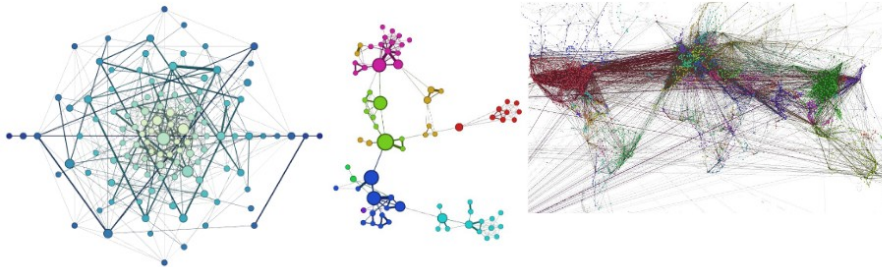
Remembering Our Classes

1 – Fundamentals of Network Science

An Introduction To Network Science



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



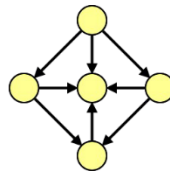
Node Properties

• Degree related metrics:

– Degree sequence

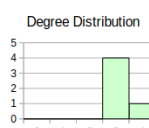
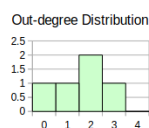
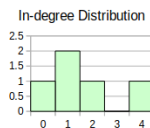
an ordered list of the (in,out) degree of each node

- 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

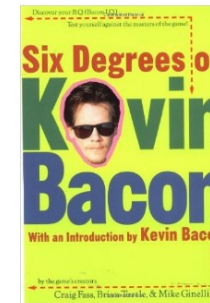
a frequency count of the occurrences of each degree
[usually plotted as probability → normalization]



Pedro Ribeiro – An Introduction to Network Science

More examples of “Small World”

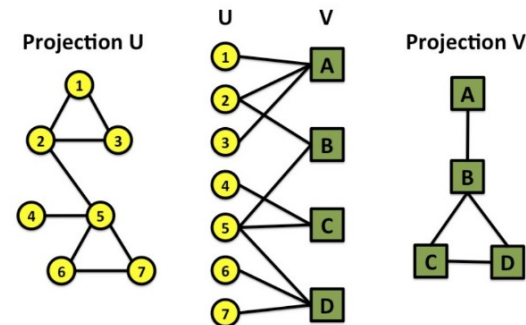
- The six degrees of Kevin Bacon
 - How many connections to link Kevin Bacon to any other actor, director, producer...
 - “Game” initiated in 1994



Pedro Ribeiro – An Introduction to Network Science

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

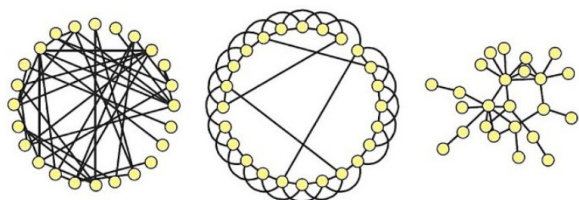
Pedro Ribeiro – An Introduction to Network Science

2 - Measuring Networks and Random Graph Models

Measuring Networks and Random Graph Models

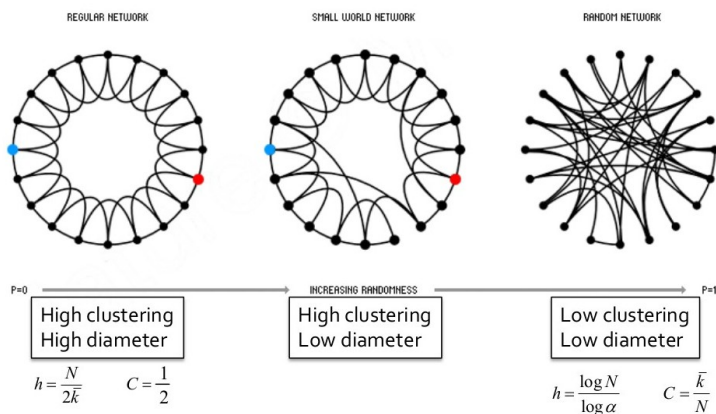


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(Heavily based on slides from Jure Leskovec and Lada Adamic@ Stanford University - CS224W)

The Small World Model



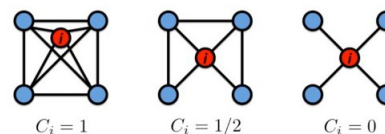
Rewiring allows us to "interpolate" between a regular lattice and a random graph

Pedro Ribeiro - Measuring Networks and Random Graph Models

(3) Clustering Coefficient

Clustering coefficient:

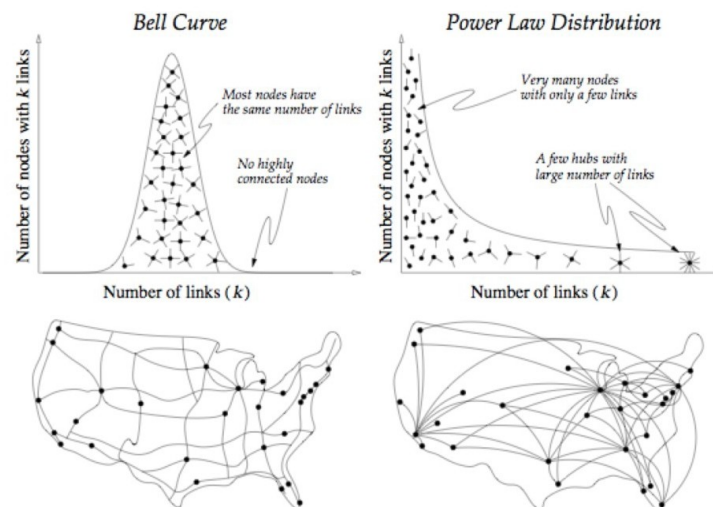
- What portion of i 's neighbors are connected?
- Node i with degree k_i
- $C_i \in [0, 1]$
- $C_i = \frac{2e_i}{k_i(k_i-1)}$ where e_i is the number of edges between the neighbors of node i



- **Average clustering coefficient:** $C = \frac{1}{N} \sum_i C_i$

Pedro Ribeiro - Measuring Networks and Random Graph Models

Interpreting Power-Laws



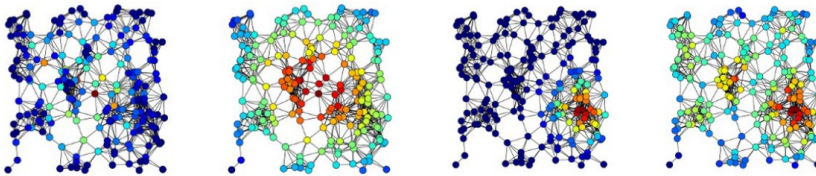
Pedro Ribeiro - Measuring Networks and Random Graph Models

3 - Node Centrality

Node Centrality



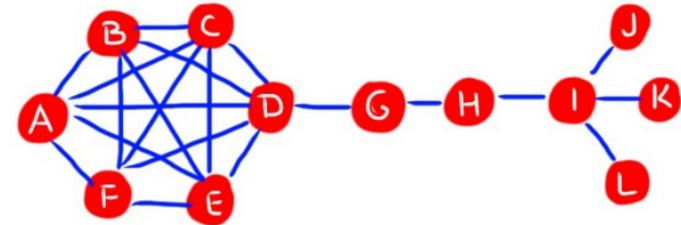
Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)



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

Betweenness: Question

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



Pedro Ribeiro - Node Centrality

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:

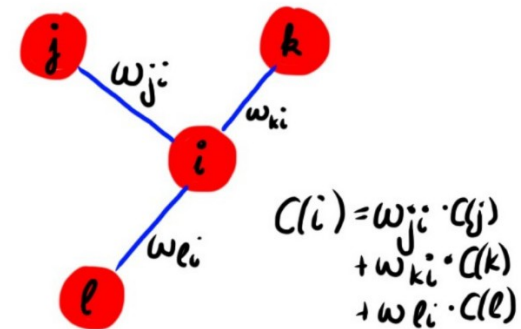
$$C'_C(i) = C_C(i) \times (n-1)$$

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

Pedro Ribeiro - Node Centrality

Eigenvector Centrality

- How “central” you are depends on how “central” your neighbors are



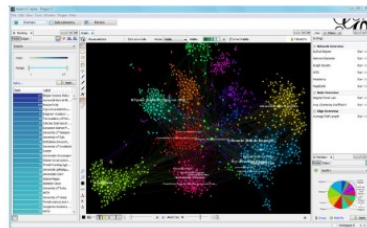
Pedro Ribeiro - Node Centrality

4 - Network Analysis and Visualization with Gephi

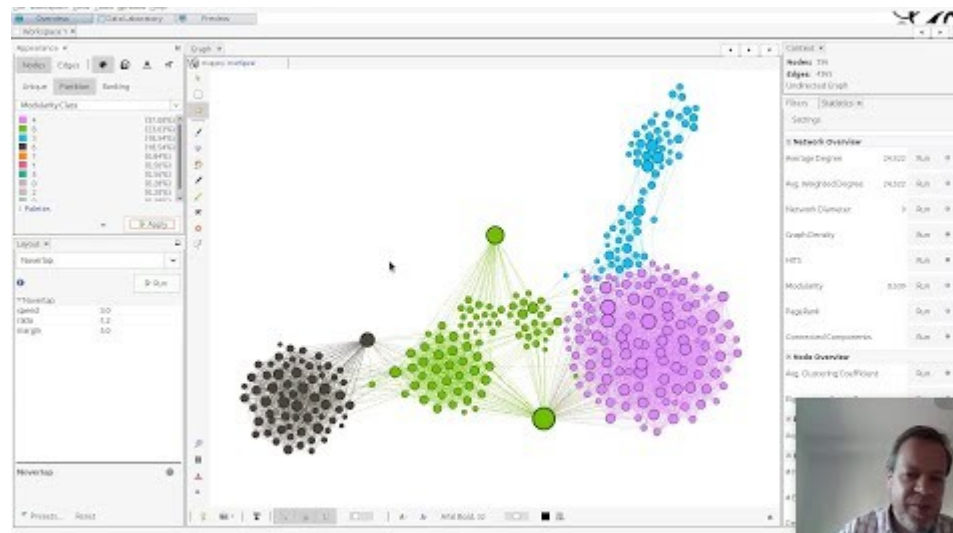
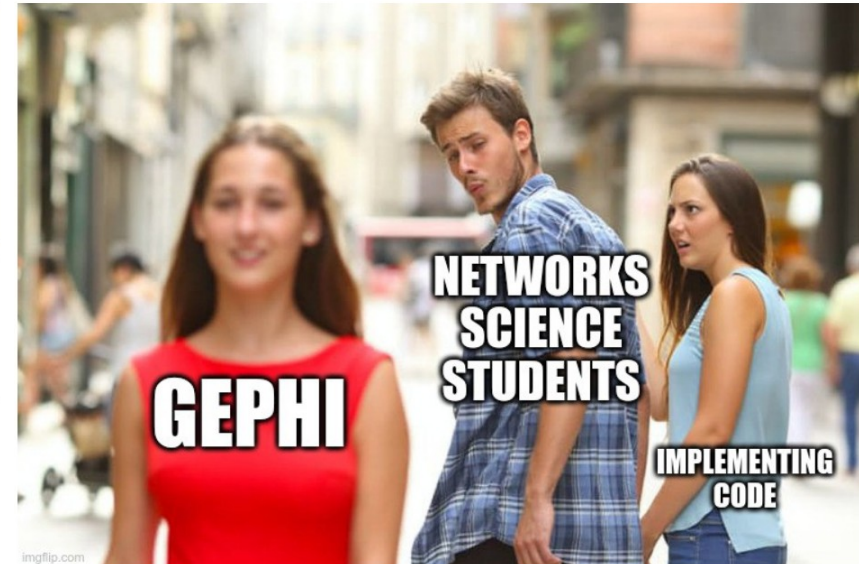
Network Analysis and Visualization with Gephi



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

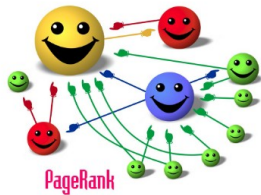


Gephi



5 - Link Analysis

Link Analysis: PageRank



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

Hubs and Authorities

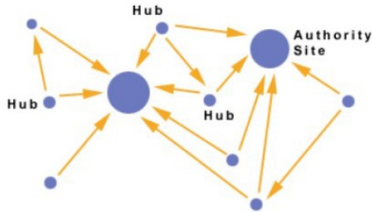
Interesting pages fall into two classes:

- 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

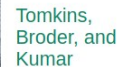


Pedro Ribeiro - Link Analysis: PageRank

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

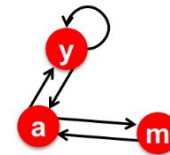


Pedro Ribeiro - Link Analysis: PageRank

PageRank: How to Solve?

- **Power Iteration:**

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



	y	a	m
y	$\frac{1}{2}$	$\frac{1}{2}$	0
a	$\frac{1}{2}$	0	1
m	0	$\frac{1}{2}$	0

$$\begin{aligned} \mathbf{r}_y &= \mathbf{r}_y/2 + \mathbf{r}_a/2 \\ \mathbf{r}_a &= \mathbf{r}_y/2 + \mathbf{r}_m \\ \mathbf{r}_m &= \mathbf{r}_a/2 \end{aligned}$$

- **Example:**

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

Iteration 0, 1, 2, ...

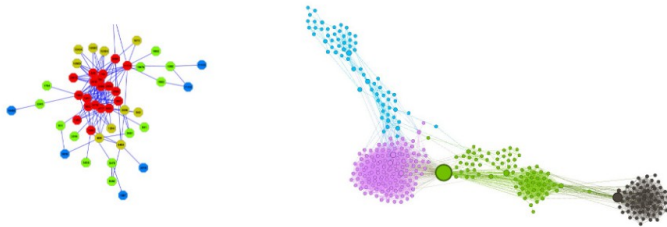
Pedro Ribeiro - Link Analysis: PageRank

6 - Roles and Community Structure in Networks

Community Structure in Networks



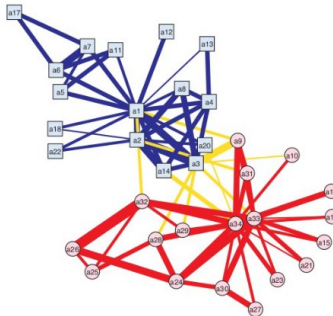
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(Mainly selected slides from Jure Leskovec and Gonzalo Mateos)

Zachary's karate club

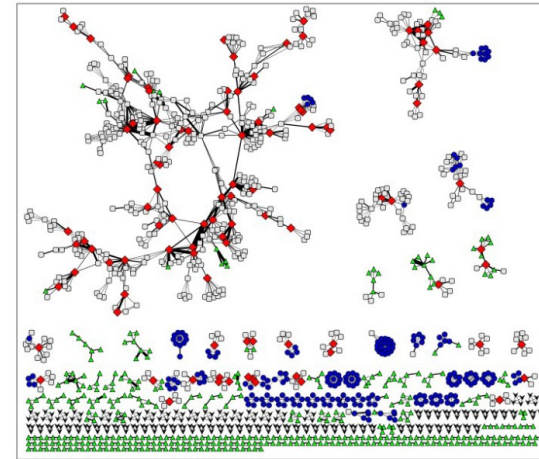
- Social interactions among members of a karate club in the 70s



- 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)

Pedro Ribeiro - Community Structure

Examples of Roles

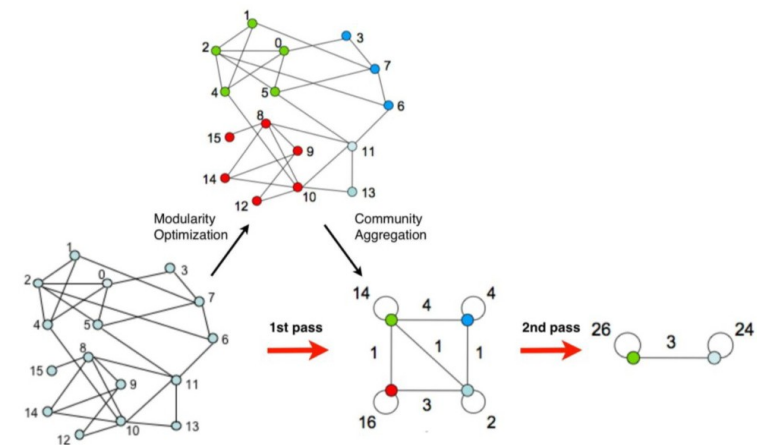


- ◆ centers of stars
- members of cliques
- ▲ peripheral nodes

Network Science
Co-authorship network
[Newman 2006]

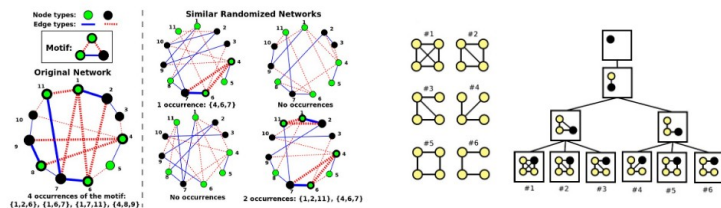
Pedro Ribeiro - Community Structure

Louvain Algorithm Overview



Pedro Ribeiro - Community Structure

7 - Subgraph Patterns



Subgraphs as Fundamental Ingredients of Complex Networks

Concepts, Methods and Applications



Pedro Ribeiro

DCC/FCUP & CRACS/INESC-TEC



Network Science (DCC/FCUP)

Subgraph concepts – Significance

Traditional Null Model – keep **Degree Sequence**

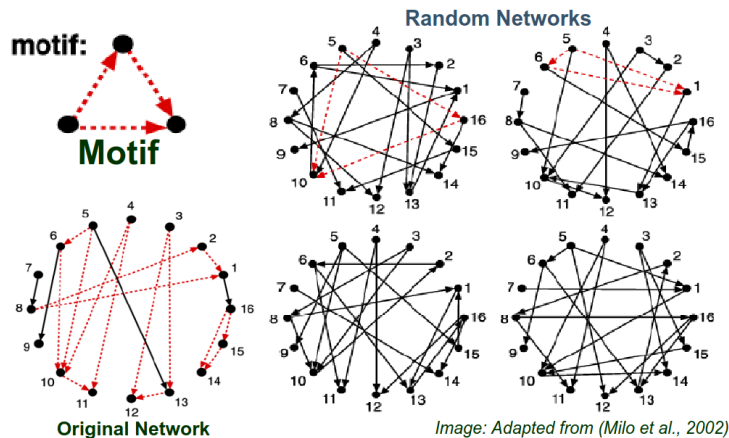
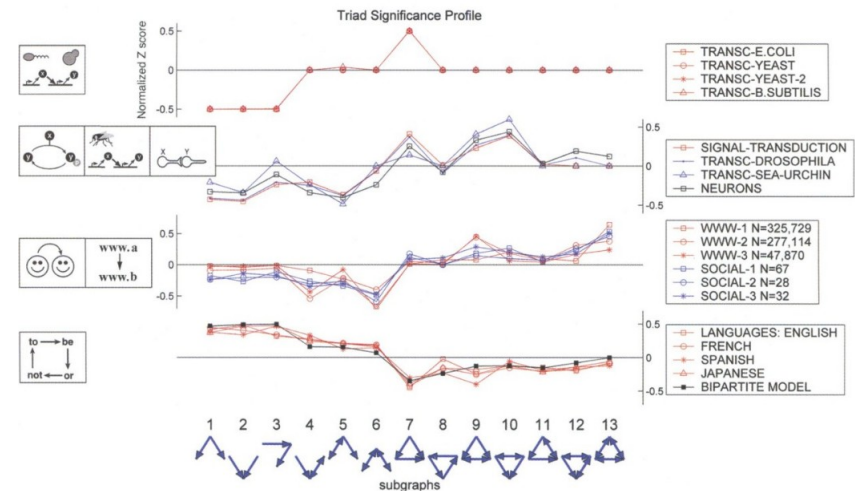


Image: Adapted from (Milo et al., 2002)

Subgraphs: fundamental ingredients of networks

Pedro Ribeiro

Example Application



Different networks have similar fingerprints!

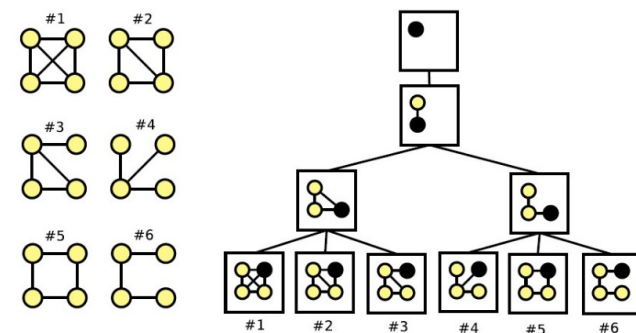
Image: (Milo et al., 2004)

Subgraphs: fundamental ingredients of networks

Pedro Ribeiro

The G-Trie data structure

- **G-Tries:** (customized) collections of subgraphs
 - **Common substructures** are identified
 - Information is “**compressed**”



[Ribeiro & Silva, DMKD, 2014]

Subgraphs: fundamental ingredients of networks

Pedro Ribeiro

8 - Analyzing networks with NetworkX



NetworkX
Network Analysis in Python

Adding edges and nodes explicitly

Here is our first example of an undirected graph:

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

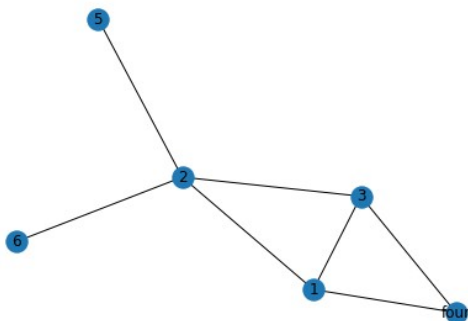
# Create some nodes
G.add_node(1)           # create a single node
G.add_nodes_from([2,3]) # create nodes from a list
G.add_node("four")      # node labels can be of different types (anything hashable)

# 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

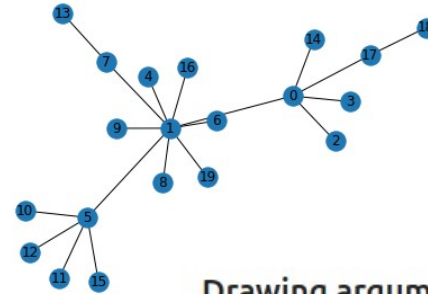
# Show nodes and edges
print(G.nodes)
print(G.edges)

# 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')]
```



```
# 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)
```

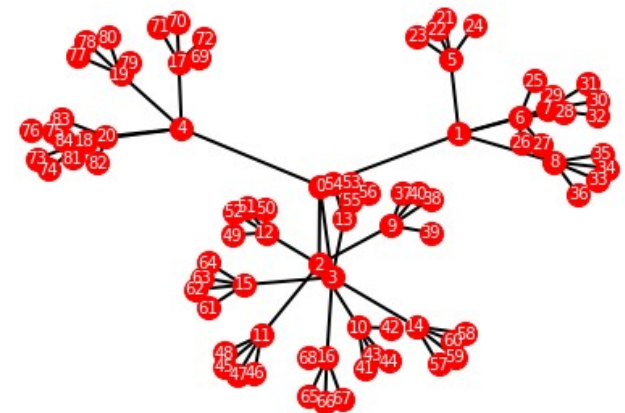


Drawing arguments

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)
    )
```

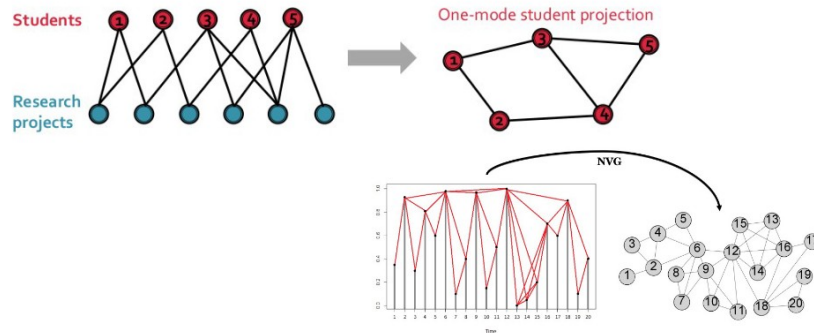


9 - Network Construction

Network Construction



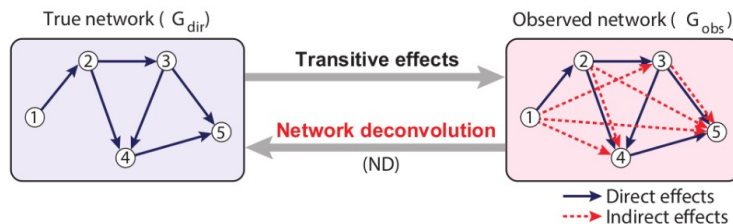
Pedro Ribeiro
(DCC/FCUP & CRACS/INESC-TEC)



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

Network Deconvolution

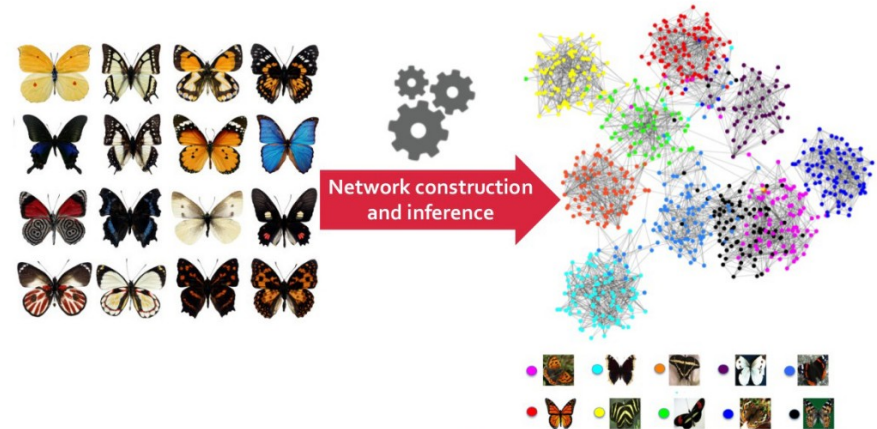
- **Goal:** Reverse the effect of transitive information flow across all indirect paths:
 - Recover **true direct network** (blue edges, G_{dir}) based on **observed network** (combined blue and red edges, G_{obs})



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

Pedro Ribeiro - Network Construction

How to construct networks?



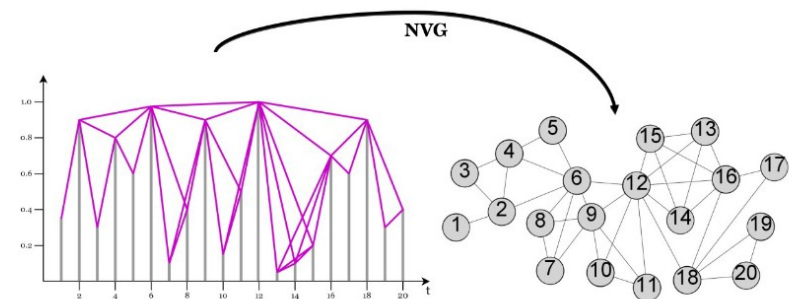
Today: **How to construct and infer networks from raw data?**

Pedro Ribeiro - Network Construction

Visibility Graphs

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

Natural Visibility Graph



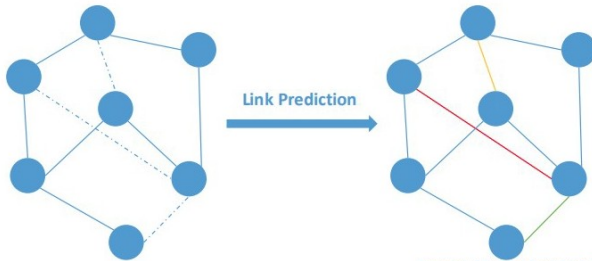
Pedro Ribeiro - Network Construction

10 - Link Prediction

Link Prediction: an introduction



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



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

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

Resource Allocation Index

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

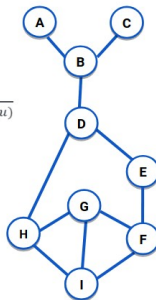
How to compute?

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

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

Example:

$$\text{res_alloc}(F, H) = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}$$



Pedro Ribeiro – Link Prediction: an introduction

Link Prediction: Methods

A Survey of Link Prediction in Complex Networks

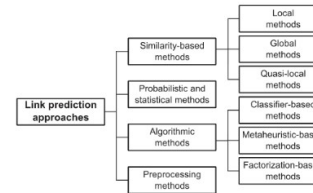
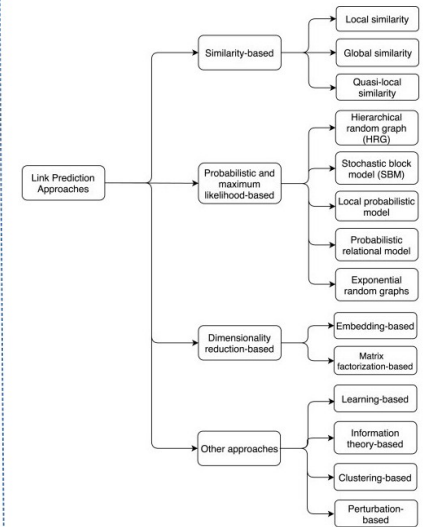


Fig. 1. Our proposed taxonomy for link prediction techniques.



Pedro Ribeiro – Link Prediction: an introduction

Community-based measures

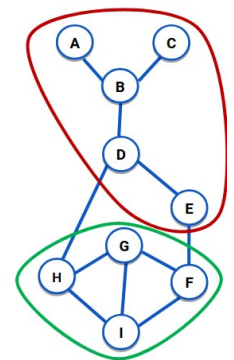
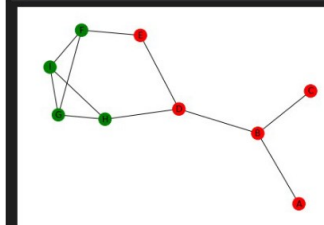
Community-based measures

```
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)
```



NetworkX
Network Analysis in Python

Pedro Ribeiro – Link Prediction: an introduction

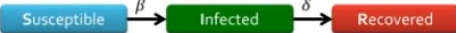
Other Material

Diffusion and Cascading Behavior

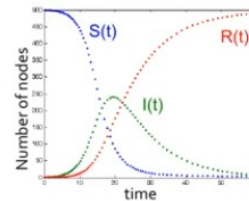
Network Effects and Cascading Behavior (1)

CS224W: Analysis of Networks
Jure Leskovec, Stanford University
<http://cs224w.stanford.edu>

SIR Model

- **SIR model:** Node goes through phases

- Models chickenpox or plague:
 - Once you heal, you can never get infected again
- Assuming perfect mixing (The network is a complete graph) the model dynamics are:

$$\frac{dS}{dt} = -\beta SI \quad \frac{dR}{dt} = \delta I$$
$$\frac{dI}{dt} = \beta SI - \delta I$$

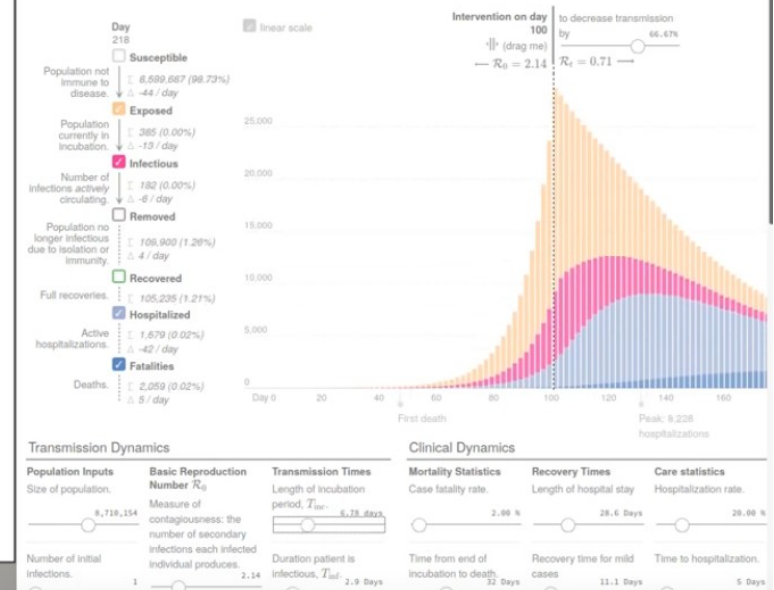


10/30/18

Jure Leskovec, Stanford CS224W: Analysis of Networks, <http://cs224w.stanford.edu>

21

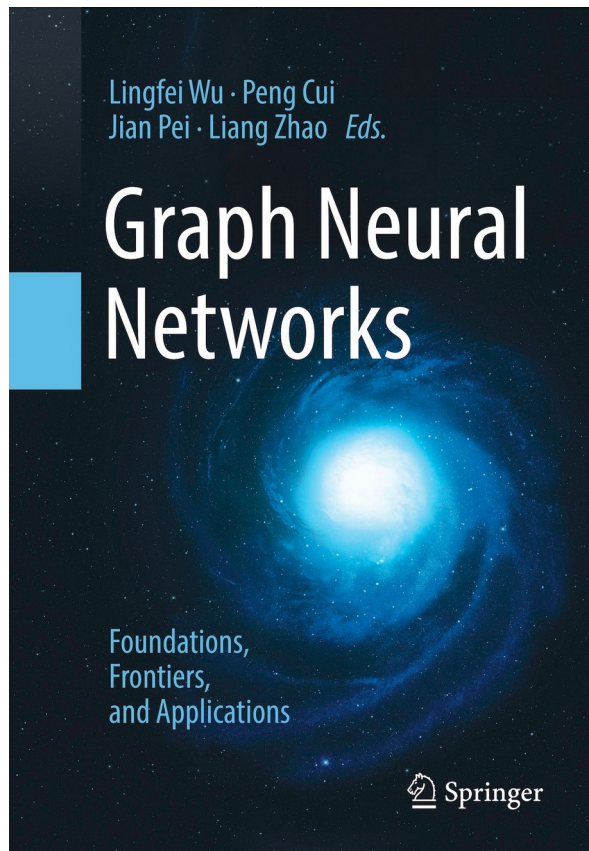
Epidemic Calculator



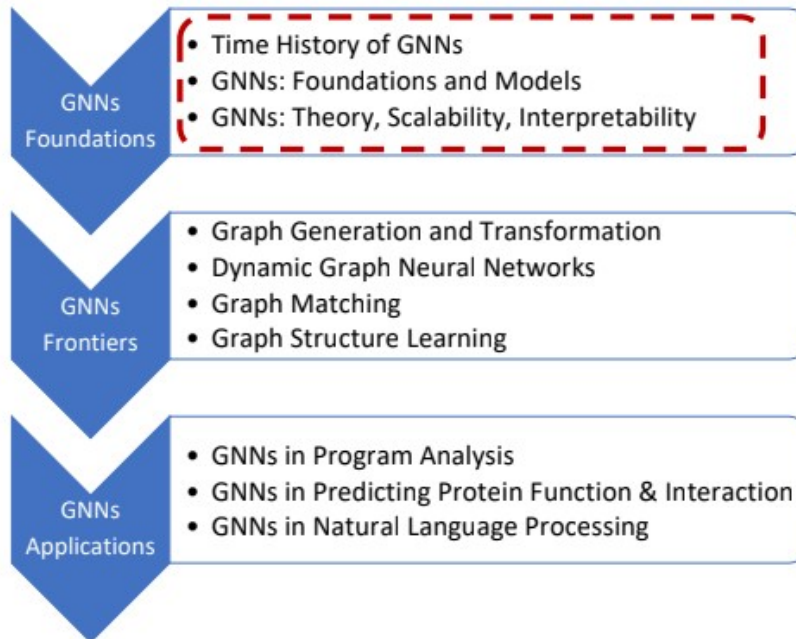
Graph Neural Networks

- “*deep learning meets network science*”

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



Outline

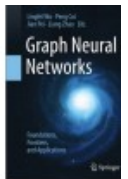


GNN book website :
<https://graph-neural-networks.github.io/index.html>

GNN Springer :
<https://link.springer.com/book/10.1007/978-981-16-6054-2>

Amazon :
<https://www.amazon.com/Graph-Neural-Networks-Foundations-Applications/dp/9811660530>

JD.com (京东商城) :
<https://item.jd.com/10043589466641.html>



2

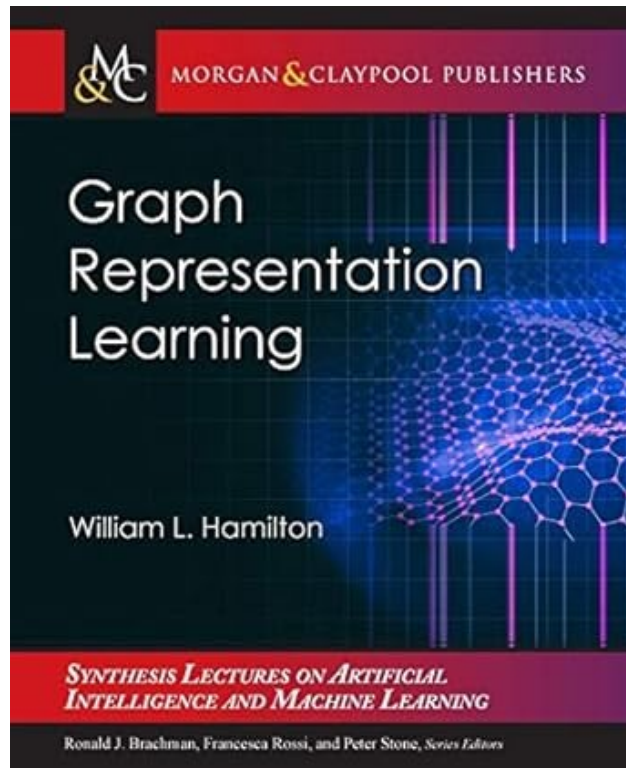


PyG



Graph Representation Learning

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



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1.1.1 Multi-relational Graphs	
1.1.2 Feature Information	
1.2 Machine learning on graphs	
1.2.1 Node classification	
1.2.2 Relation prediction	
1.2.3 Clustering and community detection	
1.2.4 Graph classification, regression, and clustering	
II Background and Traditional Approaches	
2.1 Graph Statistics and Kernel Methods	
2.1.1 Node-level statistics and features	
2.1.2 Graph-level features and graph kernels	
2.2 Neighborhood Overlap Detection	
2.2.1 Local overlap measures	
2.2.2 Global overlap measures	
2.3 Graph Laplacians and Spectral Methods	
2.3.1 Graph Laplacians	
2.3.2 Graph Cuts and Clustering	
2.3.3 Generalized spectral clustering	
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Machine Learning With Graphs

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



CS224W: Machine Learning with Graphs

Stanford / Fall 2024



Logistics

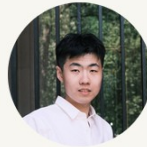
- **Lectures:** are on Tuesday/Thursday 3:00-4:20pm **in person** in the [NVIDIA Auditorium](#).
- **Lecture Videos:** are available on [Canvas](#) for all the enrolled Stanford students.
- **Public resources:** The lecture slides and assignments will be posted online as the course progresses. We are 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.
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Instructor

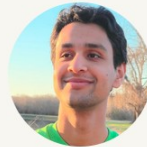


Jure Leskovec

Course Assistants



Kexin Huang (Head CA)

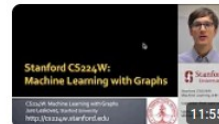


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Harper Hua

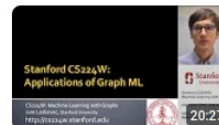
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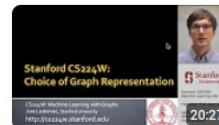
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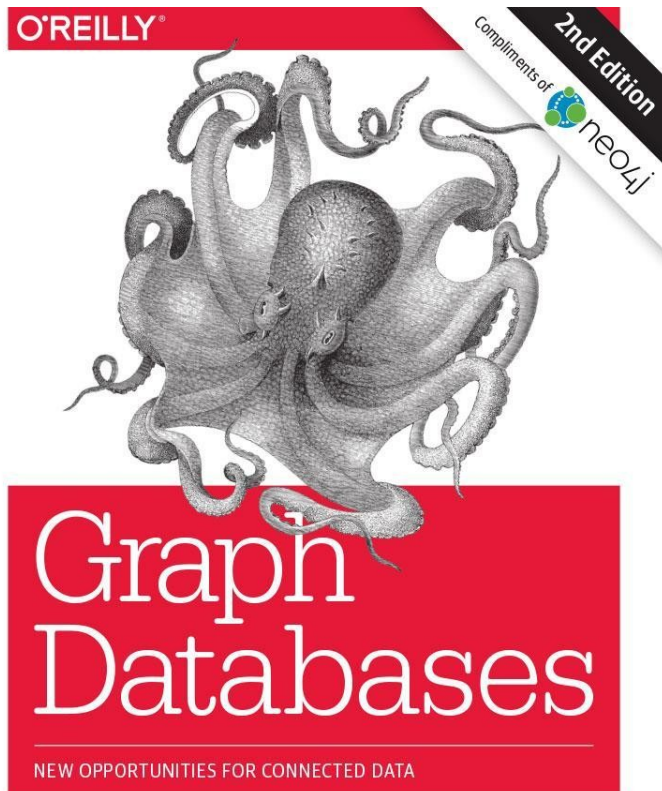


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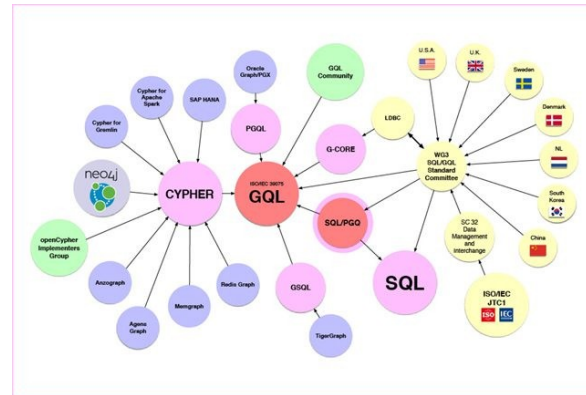
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Graph Databases

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



Ian Robinson,
Jim Webber & Emil Eifrem

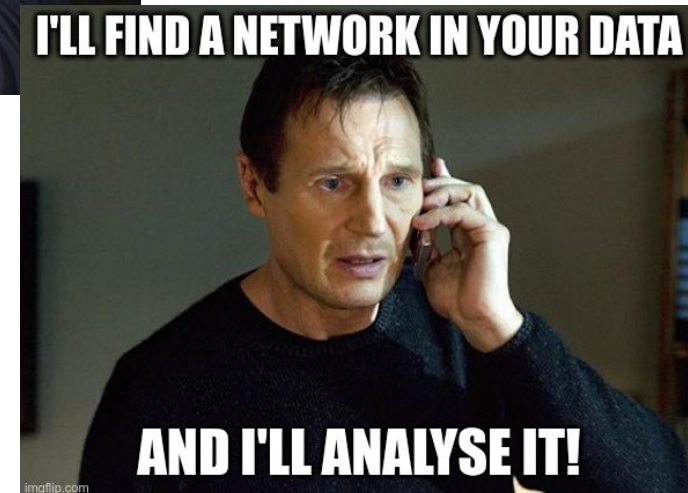


MSc Thesis in/with Network Science

Me, Myself... and Graphs!

Any
other
data types

Networks!



🎵 **Bohemian Graphsody – A Tribute to Network Science** 🎵

(To the tune of "Bohemian Rhapsody" by Queen)

[Intro – slow piano ballad]

Is this adjacency?
Is this just symmetry?
Caught in a structure
No escape from topology

Open your mind
Look to the sky and seeeee—
I'm just a node, now
I need no sympathy
Because I'm
In-degree, out-degree
Weighted edge, randomly
Any way it flows, the links really matter to me...
To meeee...

[Verse 1 – soft rock begins]

Mama, just built a graph
Put some edges in the file
Gave some weights, now watch it spiral
Mama, my code had just begun
But now I've gone and found a giant cliiiiique

Mama, ooooh...
Didn't mean to blow your mind
If I find a hub again this time tomorrow
Carry on, carry on—as if Erdős still mattered

🎵 Bohemian Graphsody – A Tribute to Network Science 🎵

(To the tune of "Bohemian Rhapsody" by Queen)

[Verse 2 – growing intensity]

Too late, my model's run
Sends a message to each friend
Through the shortest path it sends
Goodbye to random ties
I've got centrality—
Betweenness ranking's climbing up on me

Mama, ooooh (any way the flow goes...)
I can't resist this graph
I sometimes wish I'd never
seen PageRaaaaaank at all...

[Guitar Solo]

[Operatic Bridge – dramatic, many voices]

I see a little silhouetto of a node
Modularity! Modularity!
Will you do the detection?

Communities dividing, very very enlightening me!
(Oh-oh-oh) Clustering! (Oh-oh-oh) Clustering!
Clustering! Clustering! Figaro—metrics gooo!

[Heavy Rock Section]

I'm just a small node, nobody loves me
(He's just a small node in a dense community!)
Spared from isolation by connectivity!

Easy come, easy go, will this edge let it grow?
Bipartite! No, we will not let it grow! (Let it grow!)
Weighted edge! We will not let it grow! (Let it grow!)
Directed? No! (Let it grow!) Undirected? No! (Let it grow!)
Never never let it grow—oooooooo!

🎵 Bohemian Graphsody – A Tribute to Network Science 🎵

(To the tune of "Bohemian Rhapsody" by Queen)

[Breakdown – dramatic, soft then loud]

No, no, no, no, no, no, no!
Oh my modularity, my modularity!
Modularity, let me gooooooooo—
Erdős has a devil put aside for meee!
For meeeeee! For meeeeeeee!

[Finale – epic and reflective]

So you think you can cluster and leave me to cry?!
So you think you can label my node and not say why?!
Oh baby—can't do this to me baby—
Just gotta trace out, just gotta trace the whole graph here—

[Outro – soft piano, fading]

Oooh—
Nodes really matter...
Anyone can see...
Nodes really matter—
Nodes really matter...
To meeeeeeee...

(Any way the flow goes...)