

Análise de Redes

Aula 01 - Apresentação da Disciplina

Prof. Patrick Terrematte



APRESENTAÇÃO

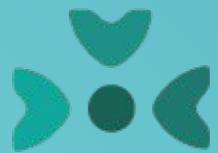
EDUCATION PRESENTATION

Formação

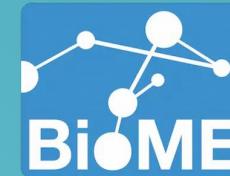
-  Bacharelado em Filosofia (UFRN, 2008)
-  Análise de sistemas (IFRN, 2011)
-  Mestrado em Sistemas e computação
(UFRN/PPgSC, 2013)
-  Doutorando em Bioinformática
(UFRN/PPgBioinfo, 2022)

Linhas de pesquisa

-  Informática Educacional e Ensino de Lógica
-  Teoria da Informação e Aprendizagem de Máquina
-  Bioinformática, Seleção de Característica,
Proteômica, Modelagem Biológica
-  Linguagens de programação:
C, Python, R, Scilab, Octave



SigSaúde



Publicações



(IEEE Access, 2169-3536, IF 3.476, Qualis A1)



dbPepVar: A Novel Cancer Proteogenomics Database

LUCAS MARQUES DA CUNHA^{1,2}, PATRICK TERREMETTE^{1,3}, TAYNÁ DA SILVA FIÚZA¹, VANDECLÉCIO LIRA DA SILVA^{1,4}, JOSÉ EDUARDO KROLL^{1,5}, SANDRO JOSÉ DE SOUZA^{1,6}, AND GUSTAVO ANTÔNIO DE SOUZA^{1,7}

(BMC Bioinformatics, 1471-2105, IF 4.341, A1)

Andrade et al. BMC Bioinformatics (2023) 24:32
<https://doi.org/10.1186/s12859-023-05155-w>

SOFTWARE

BMC Bioinformatics

Open Access



GENTLE: a novel bioinformatics tool for generating features and building classifiers from T cell repertoire cancer data

Dhiego Souto Andrade^{1*}, Patrick Terrematte¹, César Rennó-Costa^{1†}, Alona Zilberberg² and Sol Efroni^{2‡}

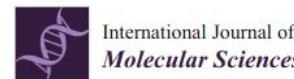
bioRxiv

Preprint

A pipeline to verify theoretical models of hypoxia signaling pathway based in Inferred Boolean Network Attractors

Alexandre Sarmento Queiroga¹, Patrick Terrematte¹, Dhiego Andrade¹, Beatriz Stransky^{1,2}, Cesar Rennó-Costa¹,

(IJMS, 1422-0067, IF 4.9, A2)



Article

Machine Learning Gene Signature to Metastatic ccRCC Based on ceRNA Network

Epitácio Farias¹, Patrick Terrematte^{2,*} and Beatriz Stransky^{1,3}



(IEEE Access, 2169-3536, IF 3.476, Qualis A1)



An Integrated Data Analysis Using Bioinformatics and Random Forest to Predict Prognosis of Patients With Squamous Cell Lung Cancer

DÉBORA V. C. LIMA¹, PATRICK TERREMETTE¹, BEATRIZ STRANSKY^{1,2}, (Member, IEEE), AND ADRIÃO D. D. NETO^{1,3}, (Senior Member, IEEE)

(Qualis A2 de Eventos em CC)

Explainable AI-driven Discovery of Staging Biomarkers in Squamous Cell Lung Carcinoma

Débora Virginia da Costa e Lima,
Bioinformatics Multidisciplinary Environment (BioME),
Metropole Digital Institute
Federal University of Rio Grande do Norte (UFRN)
Natal, Brasil
deboravlima@gmail.com

Beatriz Stransky
Bioinformatics Multidisciplinary Environment (BioME),
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Patrick Terrematte
Bioinformatics Multidisciplinary Environment (BioME),
Metropole Digital Institute
Federal University of Rio Grande do Norte (UFRN)
Natal, Brasil
patrickt@imd.ufrn.br

Adrião Duarte Dória Neto
Bioinformatics Multidisciplinary Environment (BioME),



2024

A Disciplina

- Horário para Atendimento:

- Discord: <https://discord.gg/AU53crRvhA>

- Email: patrickt@imd.ufrn.br

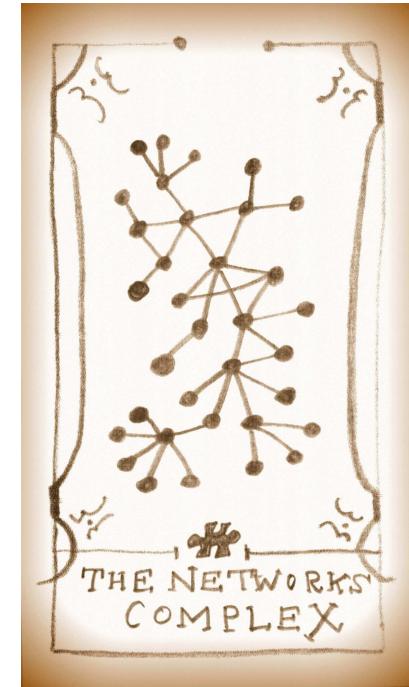
- Horário de Atendimento:

- Terças das 15h às 17h, Sala A214, sob agendamento.

- Envie email para agendar previamente

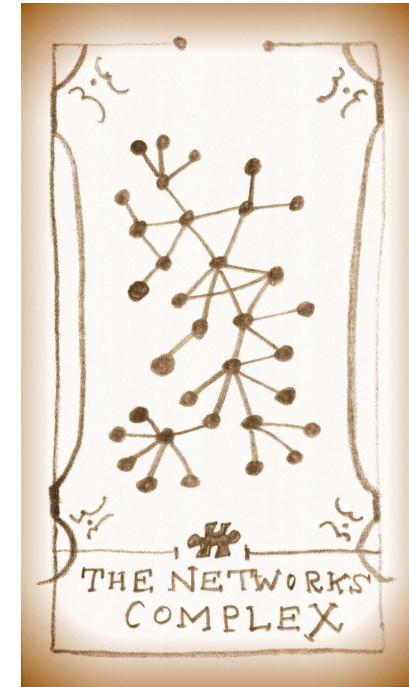
Ementa

- Elementos de redes:
 - definições básicas, densidade, esparsidade, subredes, graus, e representações.
- Small worlds
 - Assortatividade, Caminhos, Distâncias, Componentes de conexões, Coeficientes de clustering.
- Hubs
 - Distribuições de centralidade, Decomposição, Betweenness, Eigenvector Centrality.
- Aplicações
 - Estudo de caso da Wikipedia
 - Estudo de caso do Twitter



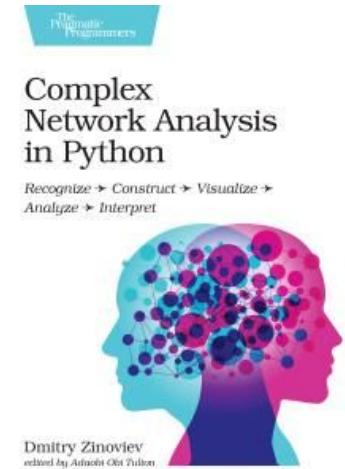
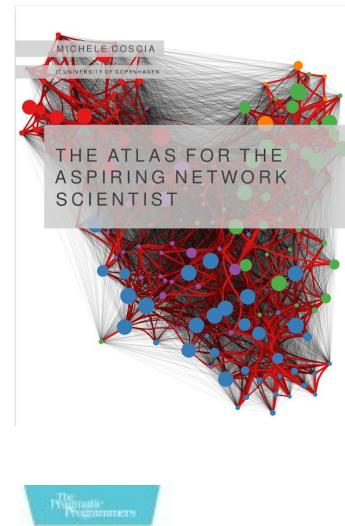
Ementa

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Referências

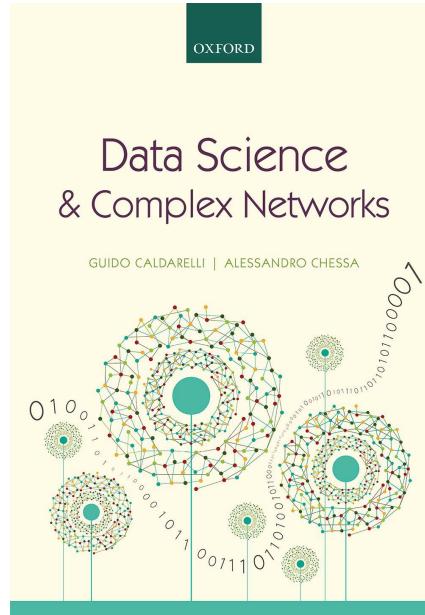
- The Atlas for the Aspiring Network Scientist, 2021
 - <https://www.networkatlas.eu/index.htm>
- Complex Network Analysis in Python, 2018
 - <https://pragprog.com/titles/dzcnapy/complex-network-analysis-in-python/>



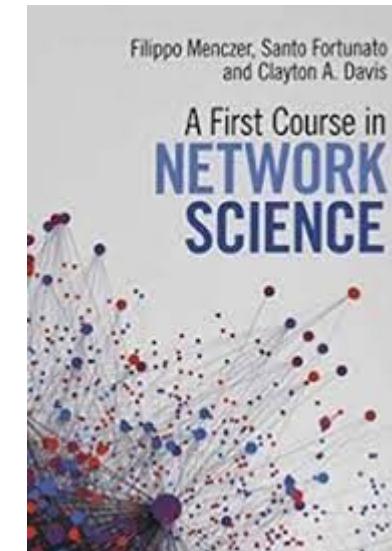
Referências

- Network Science by Albert-László Barabási
<http://networksciencebook.com/>
- Network Analysis Course – Prof. Ivanovitch (DCA/UFRN)
YouTube Playlist

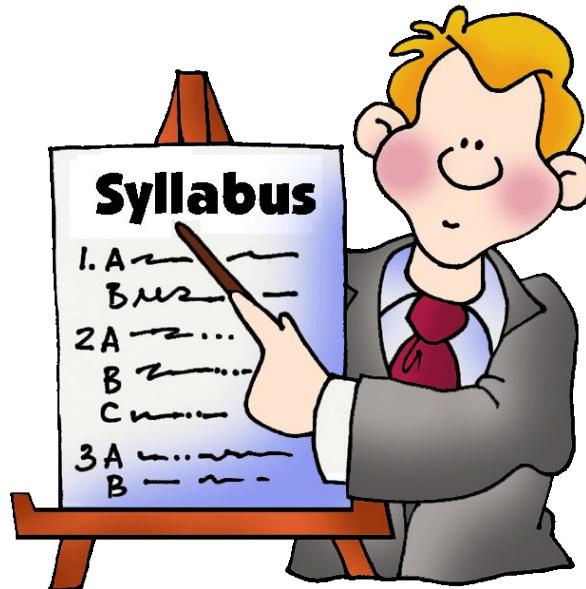
Referências



- Caldarelli, Guido; Chessa, Alessandro. **Data science and complex networks - Real cases studies with Python**, 2016.
 - Filippo Menczer; Santo Fortunato; Clayton A. Davis. **A First Course in Network Science**, 2020.



General Outline



Unidade 1: **The Architecture of Complex Networks**

Networks and Graphs
Random graphs
It's a Small world
Scale Free Networks
Centrality & Assortative Mixing
Tie Strength & Resilience
High-order Network Analysis

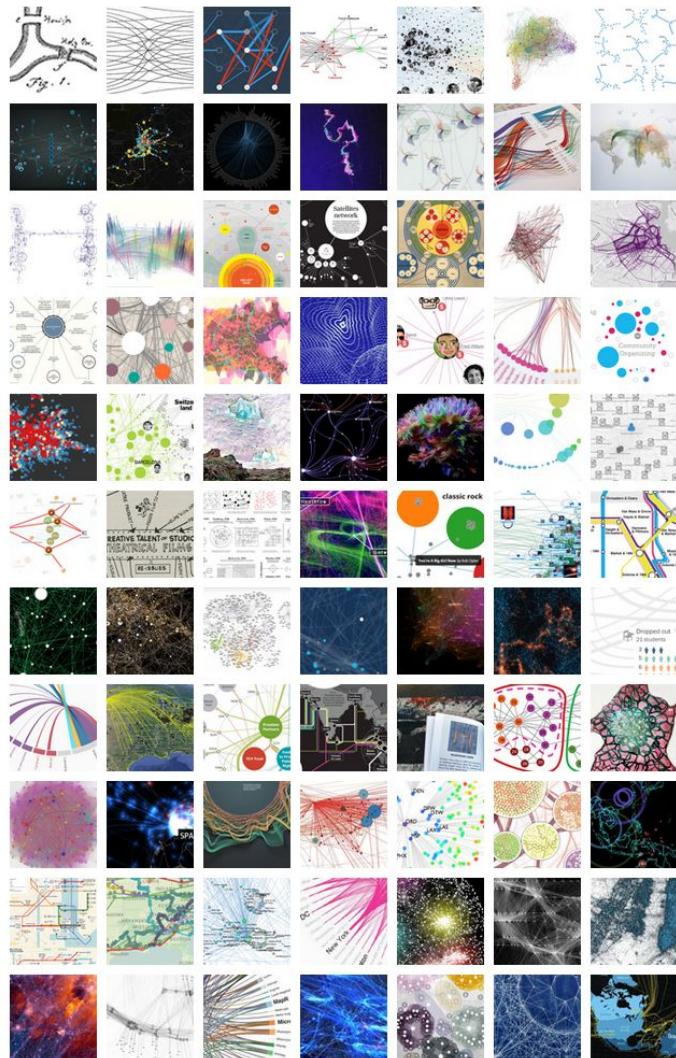
Unidade 2 **The Dynamics of Complex Networks**

Community Discovery
Dynamic of networks
Link Prediction
Dynamic Community Discovery
Diffusion: Decision based models
Diffusion: Epidemics
Diffusion: Opinion Dynamics

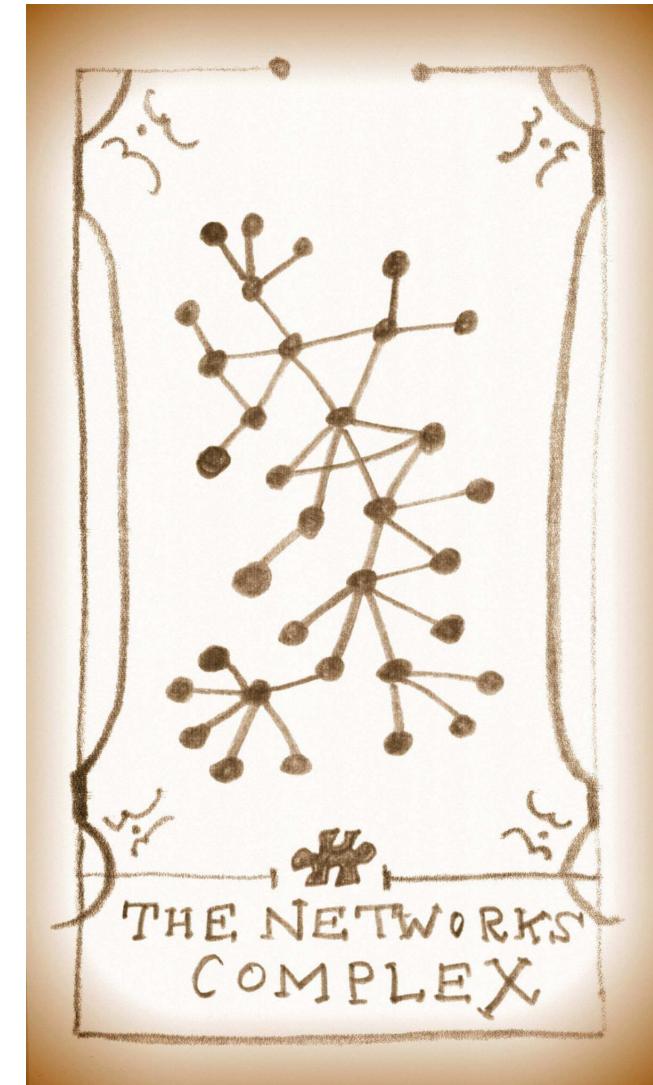
Hands-On
- Python
- Gephi & Cytoscape

Unidade 3: **Case Studies**

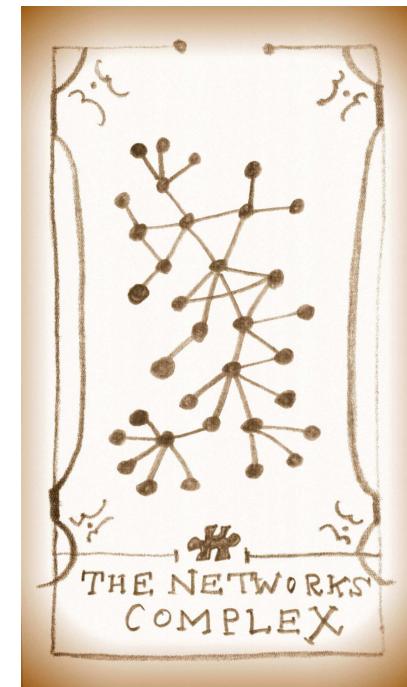
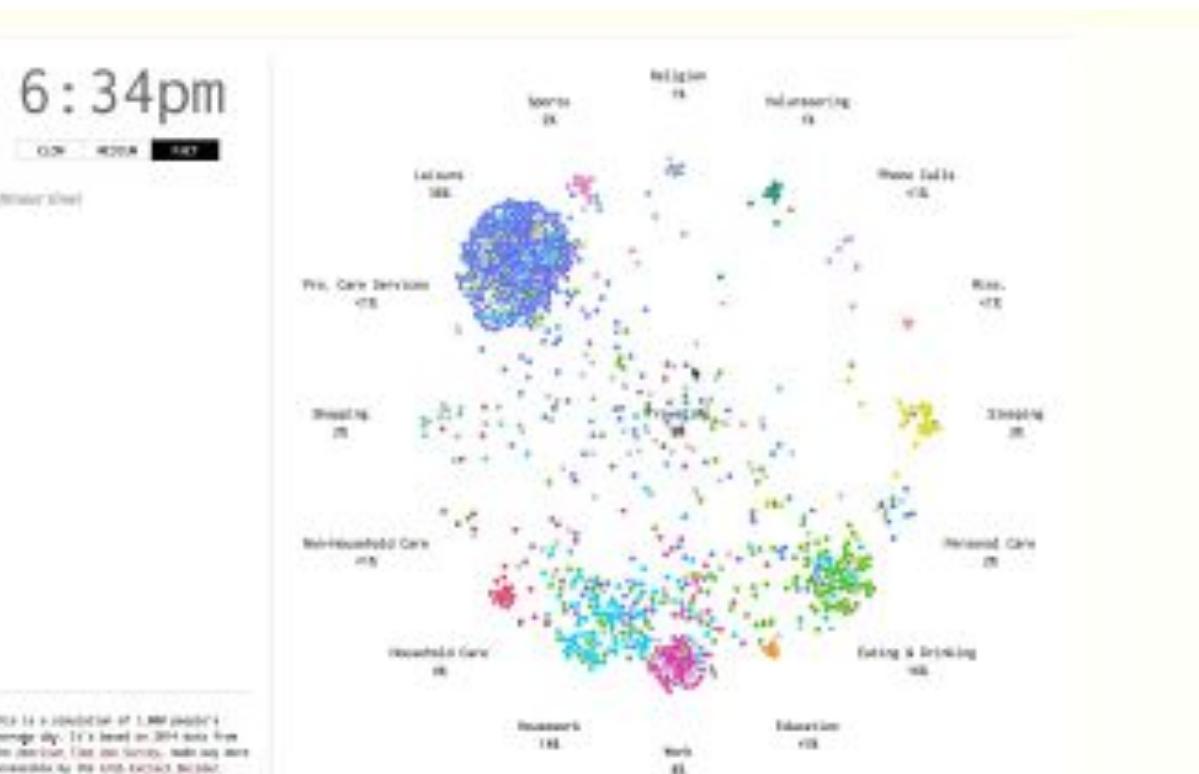
Redes Complexas



<http://www.visualcomplexity.com/vc/>



Redes Complexas



<http://flowingdata.com/2015/12/15/a-day-in-the-life-of-americans>

Datacamp

- <https://app.datacamp.com/workspace/templates/playbook-python-network-analysis>
- <https://app.datacamp.com/workspace/templates/template-python-visualize-twitter-network?selectedLabels=%5B%22network%20analysis%22%5D>



Biologia de Sistemas como aplicação de Teoria dos Grafos

*"The **reductionist approach** has successfully identified most of the components and many of the interactions but, unfortunately, offers **no convincing concepts** or methods to understand **how system properties emerge**..."*

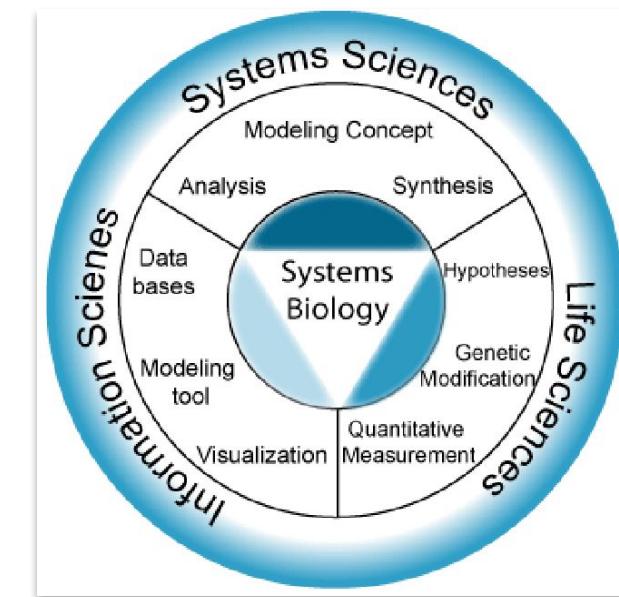
Sauer et al., 2007

*"**Systems biology**...is about **putting together** rather than taking apart, integration rather than reduction. It requires that we develop ways of **thinking about integration** that are as rigorous as our reductionist programmes, but different....It means changing our philosophy, in the full sense of the term."*

Denis Noble, 2006

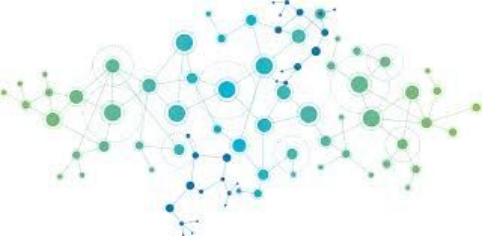
Biologia de Sistemas como aplicação de Teoria dos Grafos

- Grande quantidade de **dados experimentais**.
- Proposição de **modelos matemáticos** que explicam aspectos significativos dos dados.
- **Simulações computacionais** e análises numéricas.
- Avaliação da qualidade do modelo por comparação dos resultados com dados experimentais.



Teoria de Grafos

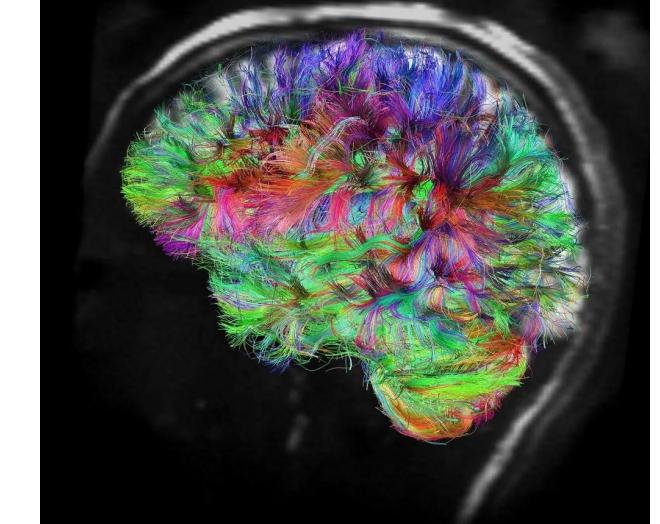
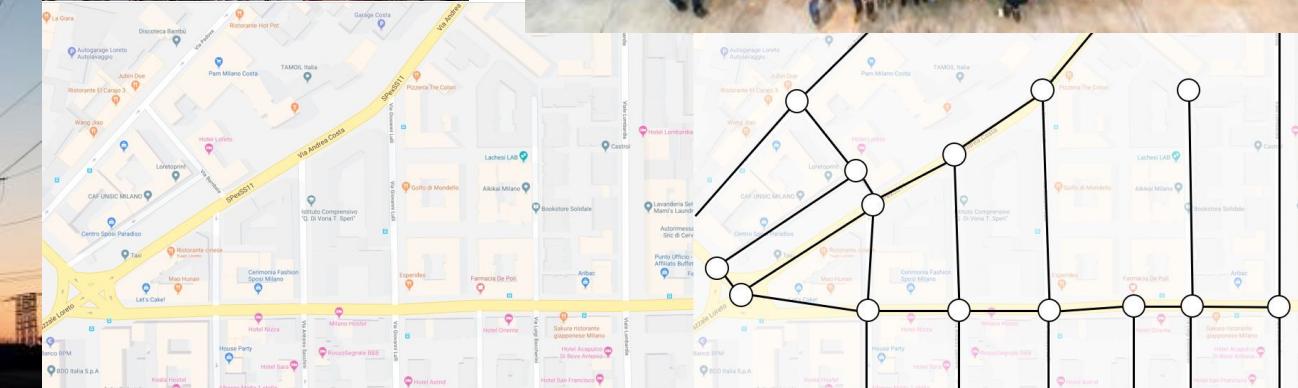
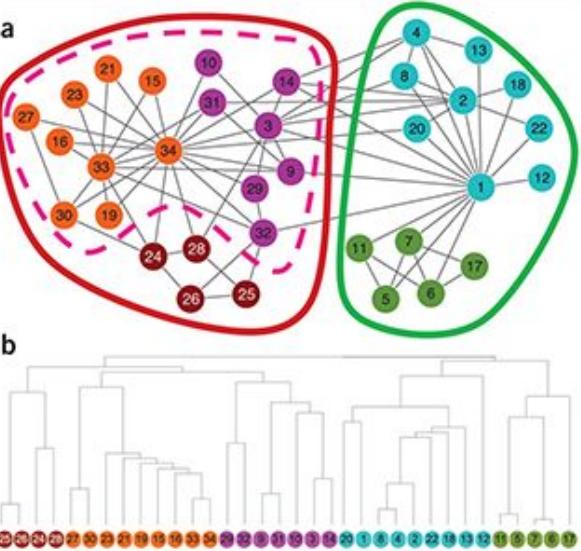
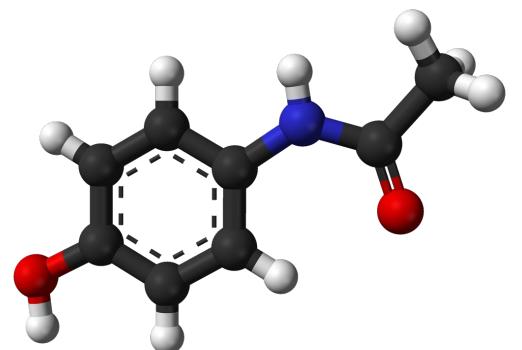
- Propriedades
 - Ordem e Tamanho
 - Caminhos e medidas
 - Grau e Distribuição de Grau
 - Coeficiente de Clusterização
 - Medidas de Centralidade
- Tipos de Redes
 - Redes Aleatórias
 - Redes 'Mundo Pequeno' (*Small Worlds*)
 - Redes Livre de Escala



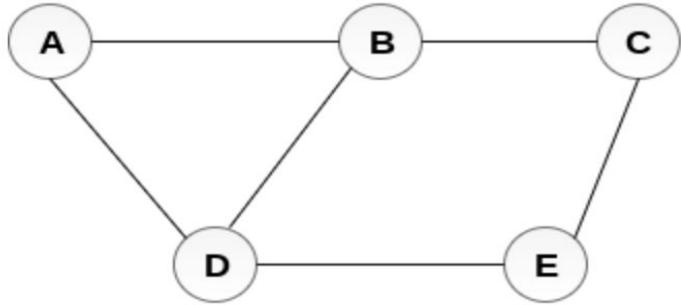
Teoria dos Grafos



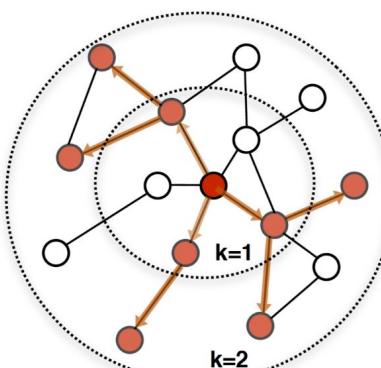
Everything is Connected!



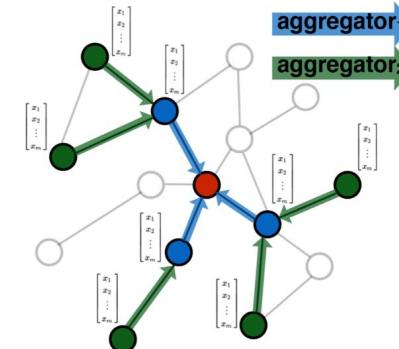
Graphs



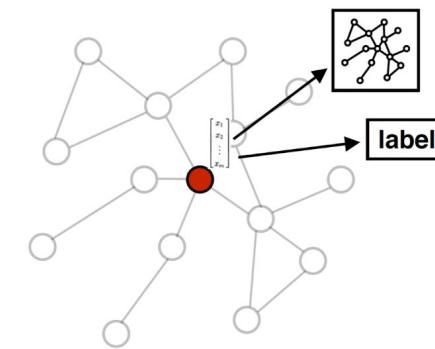
	A	B	C	D	E
A	0	1	0	1	0
B	1	0	1	1	0
C	0	1	0	0	1
D	1	1	0	0	1
E	0	0	1	1	0



1. Sample neighborhood



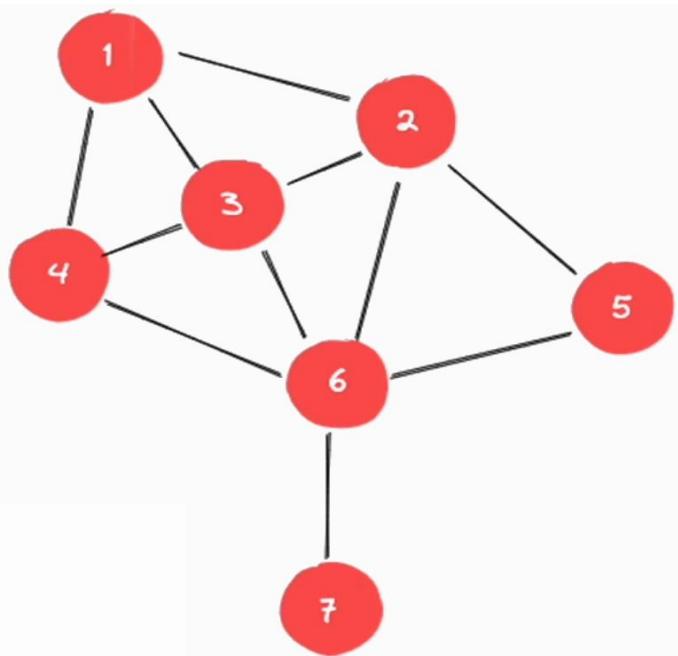
2. Aggregate feature information from neighbors



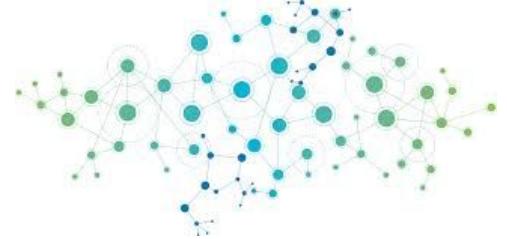
3. Predict graph context and label using aggregated information

source: snap.stanford.edu/graphsage

Caminho



Adjacent Matrix (A)								A^2							
0	1	1	1	0	0	0	0	3	1	2	1	1	3	0	0
1	0	1	0	1	1	1	0	1	4	2	3	1	2	1	0
1	1	0	1	0	1	0	0	2	2	4	2	2	2	1	0
1	0	1	0	0	0	1	0	1	3	2	3	1	1	1	0
0	1	0	0	0	1	0	0	1	1	2	1	2	1	1	0
0	1	1	1	1	0	1	0	3	2	2	1	1	5	0	0
0	0	0	0	0	1	0	0	0	1	1	1	1	0	1	0

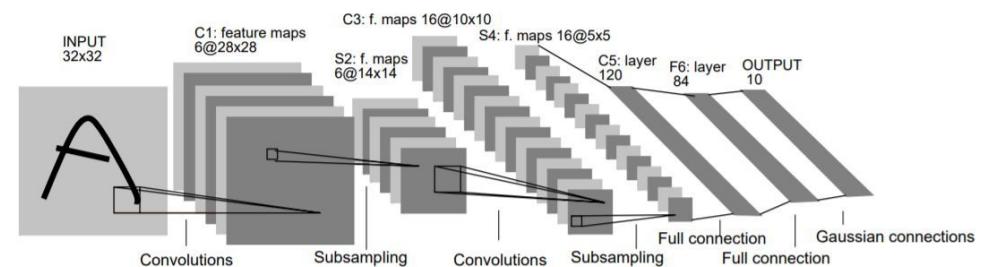
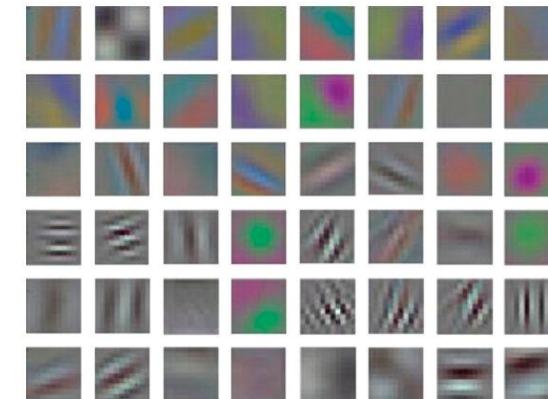
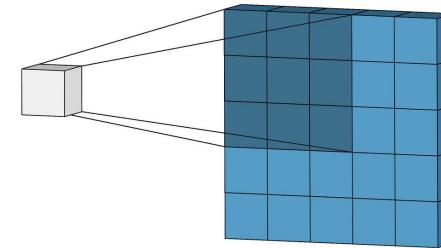


Deep Learning e Graph Neural Network

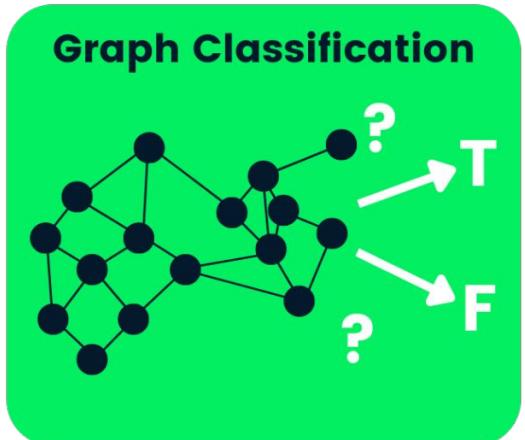


Convolutional Neural Network (CNN)

- locality
- aggregation
- composition



Learning tasks on graphs



source: datacamp.com/portfolio/kingabzpro

Chapter 1

Why should we care about Complex Networks?

Summary

- Complexity
- Real world networks
- Emergence of Network Science

Reading

- Chapter 1 & 2 of Kleinberg's book
- Chapter 1 of Barabasi's book.
- Complexity Explained



Complex

[adj., v. kuh m-pleks, kom-pleks; n. kom-pleks]
adjective

1. Composed of many **interconnected parts**; compound; composite: a complex highway system.
2. Characterized by a very complicated or involved arrangement of parts, units, etc.: complex machinery.
3. So complicated or intricate as to be hard to understand or deal with: a complex problem.

Source: Dictionary.com

Complexity, a **scientific theory** which asserts that some systems display behavioral phenomena that are completely inexplicable by any conventional analysis of the systems' constituent parts. These phenomena, commonly referred to as **emergent behaviour**, seem to occur in many complex systems involving living organisms, such as a stock market or the human brain.

Source: John L. Casti, Encyclopædia Britannica

Complexity

Behind each **complex system**
there is a **network**,
that defines the interactions
between the **components**.

Suggested Reading

Complexity Explained

<https://complexityexplained.github.io/>



Examples of

Complex Systems

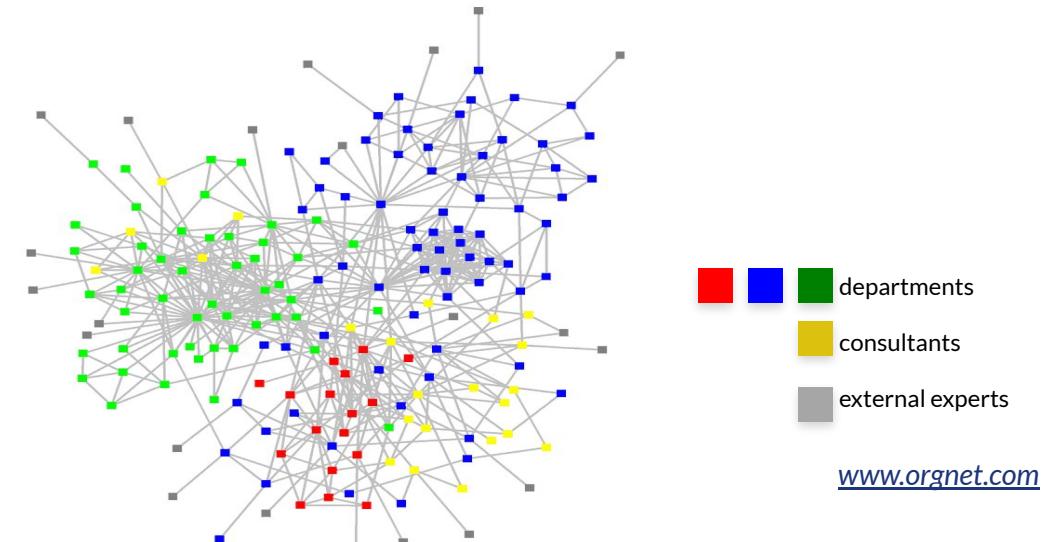
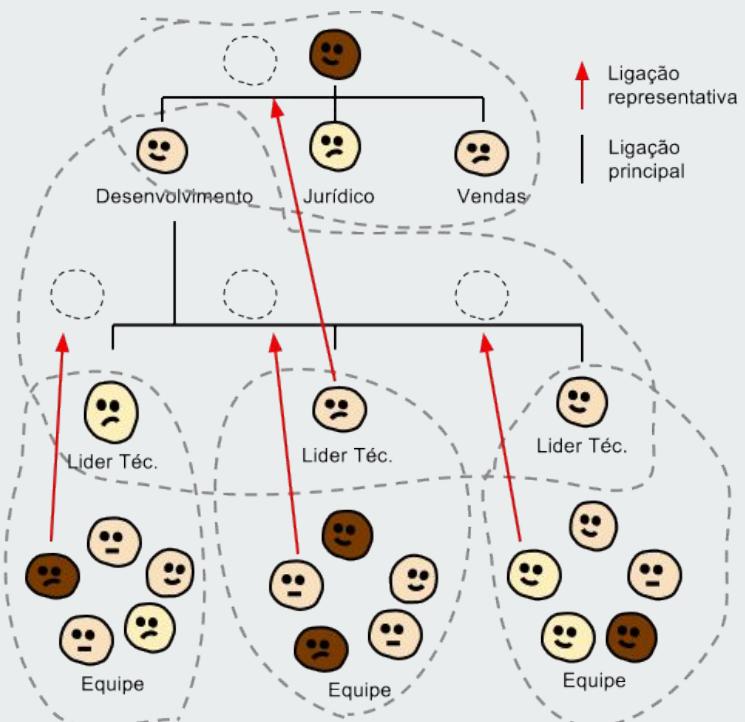
The Facebook “Social Graph”



Keith Shepherd's "Sunday Best".
<http://baseballart.com/2010/07/shades-of-greatness-a-story-that-needed-to-be-told/>

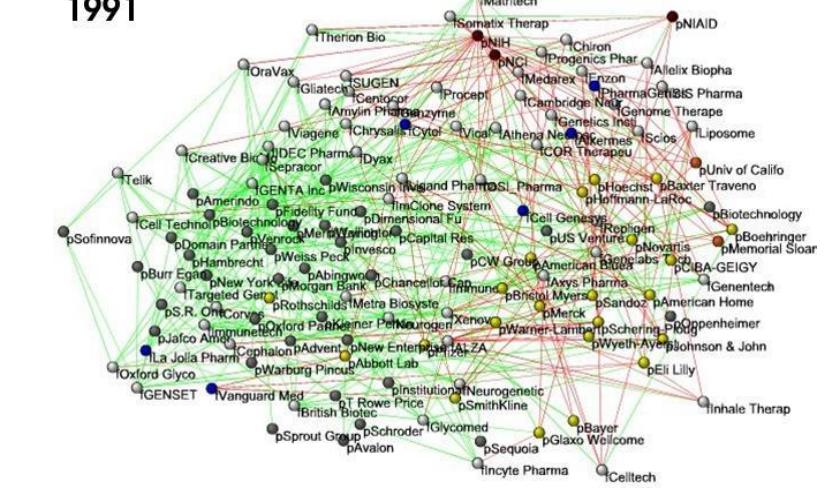
Examples of Complex Systems

The structure of an organization



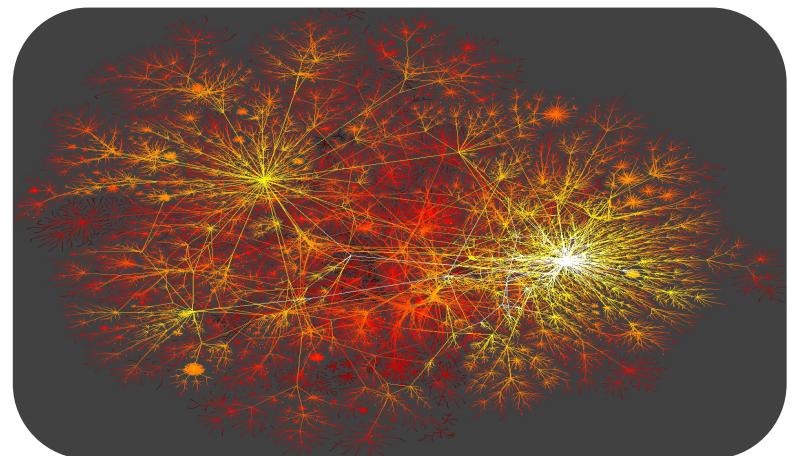
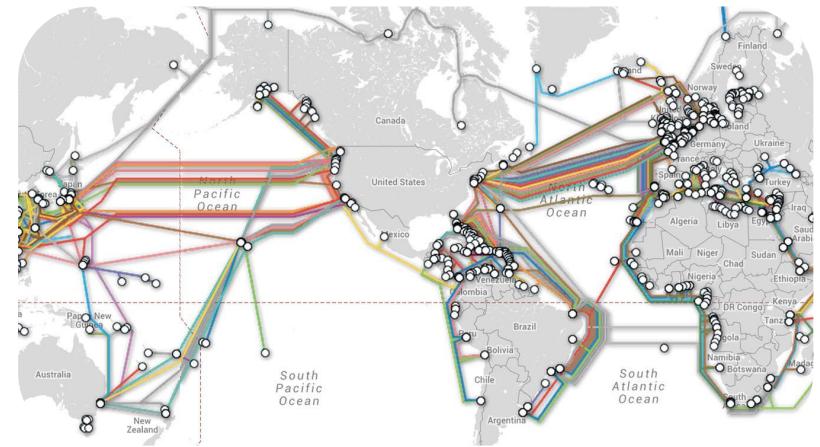
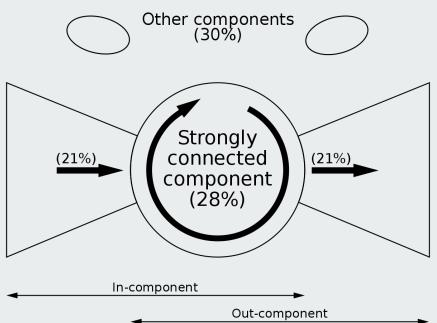
- Links:**
- Collaborations
 - Financial
 - R&D
- Nodes:**
- Companies
 - Investment
 - Pharma
 - Research Labs
 - Public
 - Biotechnology

1991



Examples of **Complex Systems**

The Internet backbone,
The World Wide Web...



Examples of

Complex Systems

Human Genes

Humans have only about three times as many genes as the fly, so human complexity seems unlikely to come from a sheer quantity of genes.

Rather, some scientists suggest, each human has a network with different parts like genes, proteins and groups.

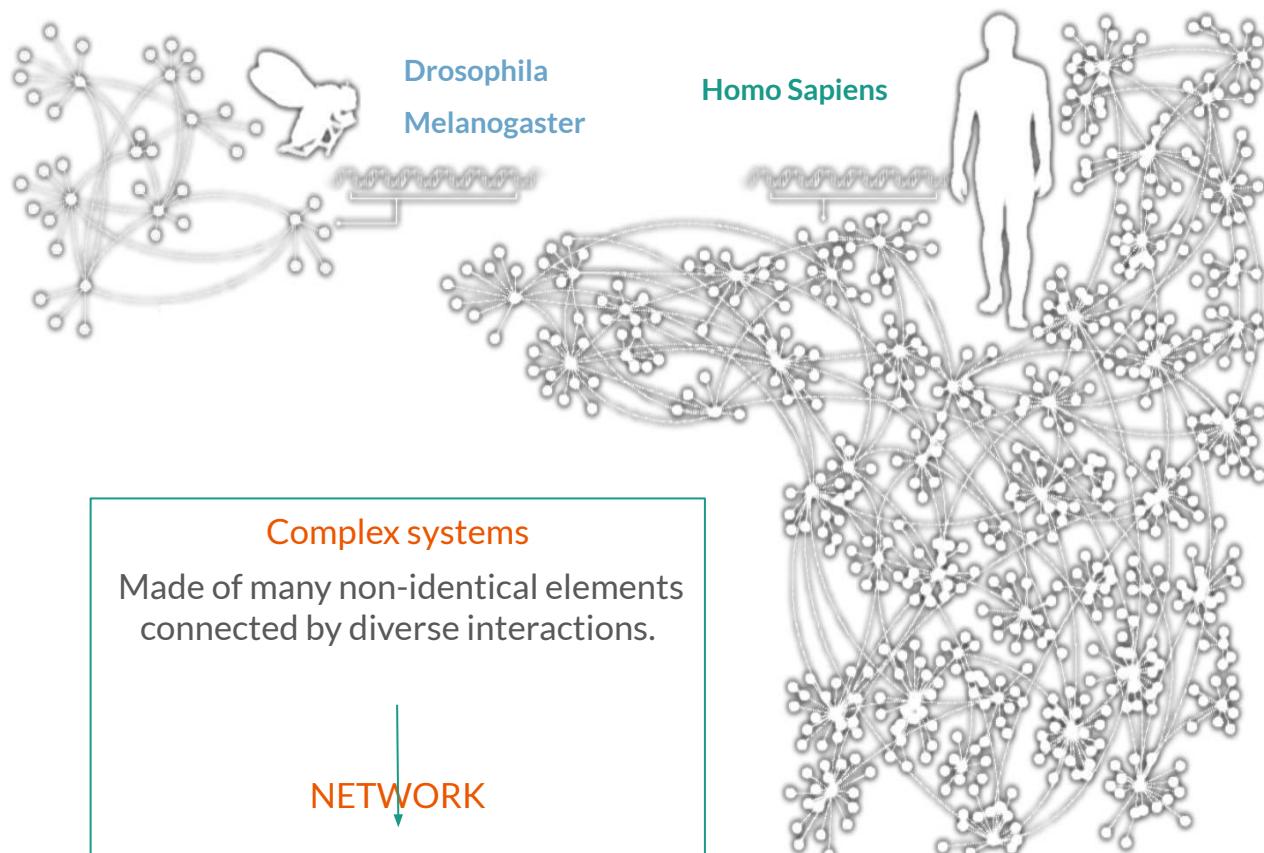


Examples of

Complex Systems

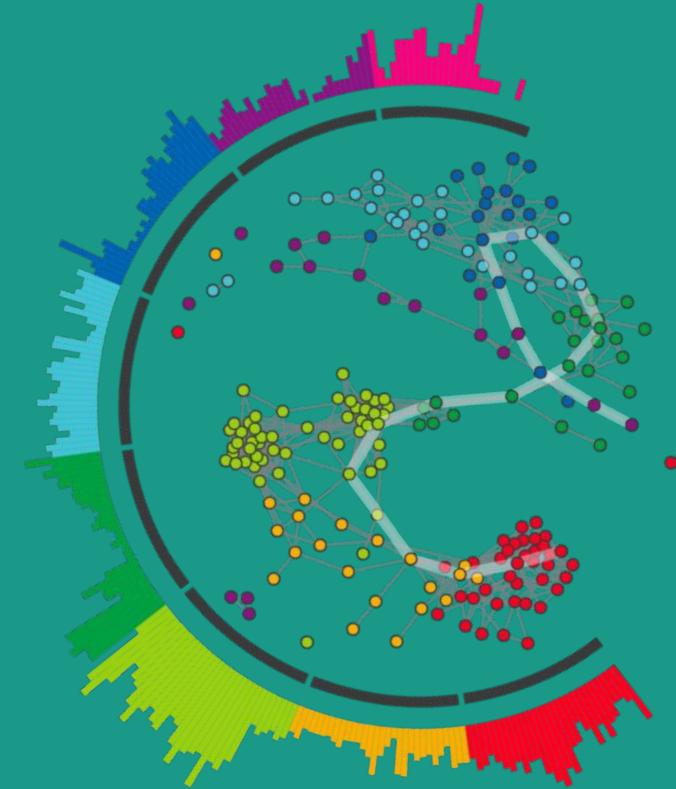
Human Genes (cont'd)

In the generic networks shown, the points represent the elements of each organism's genetic network, and the dotted lines show the interactions between them.



The role of networks

Behind each system studied in complexity there is an intricate wiring diagram, or a **network**, that defines the interactions between the component.



We will never understand **complex system** unless we map out and understand the networks behind them.



Examples of

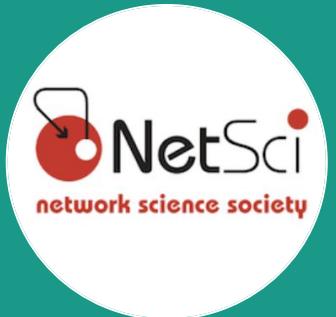
Real world Networks



Type: Social
Nodes: Individuals
Links: Social relationship



Type: Actor connectivity
Nodes: Actors
Links: Cast jointly



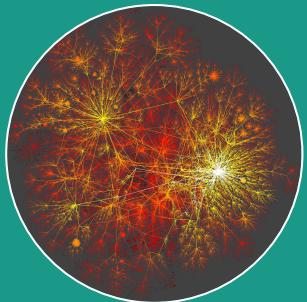
Type: Scientific Collaborations
Nodes: Researchers
Links: Co-Authorships



Type: Communication
Nodes: Phones, Airports..
Links: Phone calls, Flights..

Examples of

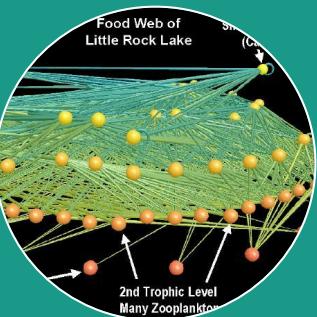
Real world Networks (cont'd)



Type: Technological
Nodes: PC, Routers
Links: Physical lines



Type: Scientific Citation
Nodes: Papers
Links: Citations



Type: Biological
Nodes: Species
Links: Trophic interactions



Type: Mobility
Nodes: Individuals, Cars...
Links: Co-Location...

The Emergence of Network Science

The (urgent) need to understand complexity

Despite the challenges complex systems offer us, we cannot afford to not address their behavior, a view increasingly shared both by scientists and policy makers.

Networks are not only essential for this journey, but during the past decade some of the most important advances towards understanding complexity were provided in context of network theory.

Data Availability

- 1990 C. elegans neural wiring diagram
- 1998 - Movie Actor Network
- 1998 - Citation Networks
- 1999 -World Wide Web
- 2000 - Metabolic Networks
- 2001 - PPI network
- 2008 - OSNs

Universality

The architecture of networks emerging in various domains of science, nature, and technology are more similar to each other than one would have expected.

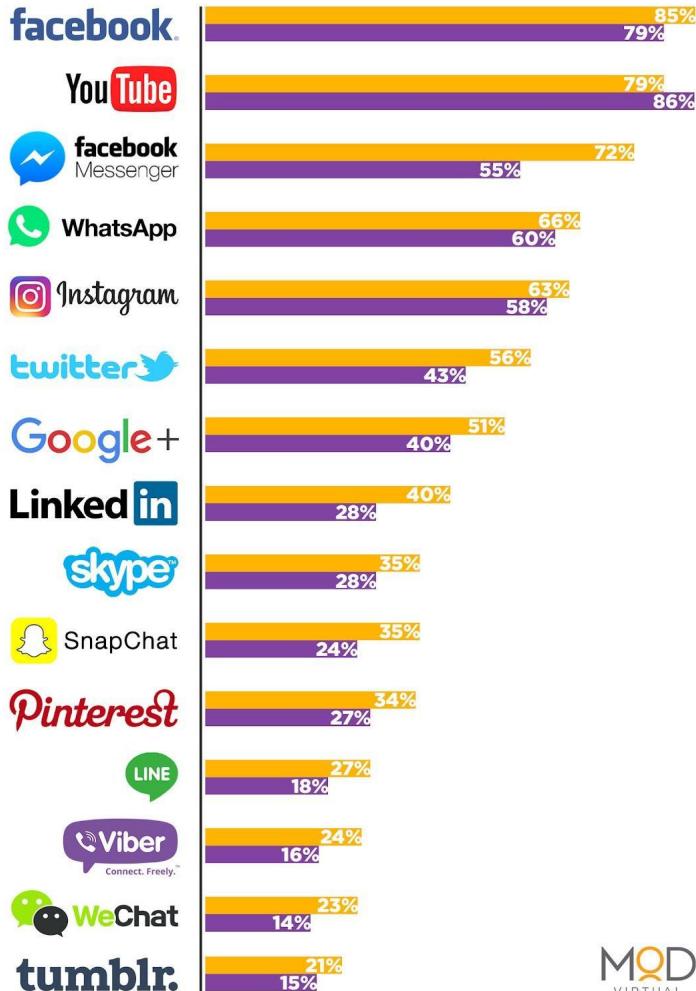


The Life of Networks



TOP 15 MOST POPULAR SOCIAL NETWORKS

MEMBERS / REGISTERED USERS VISISTORS / ACTIVE USERS



Source: GlobalWebIndex - Flagship Report 2018 | Survey Base: 98,011 Internet users aged 16-64 from outside China (Q3 2018) | digitalinformationworld.com

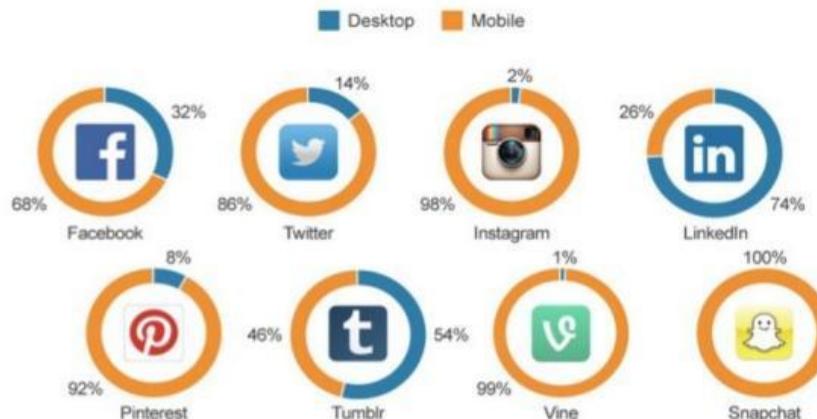
(Online) Social Networks

Time Spent on Social Media...

<http://www.statista.com/chart/2109/time-spent-on-social-networks-by-platform/>

Most Social Networks Are Now Mobile-First

% of time spent on social networks in the United States, by platform*

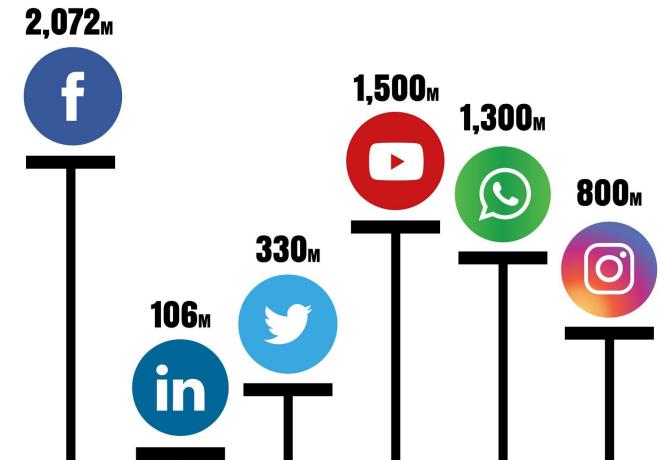


THE WALL STREET JOURNAL. * December 2013, Age 18+

Source: comScore

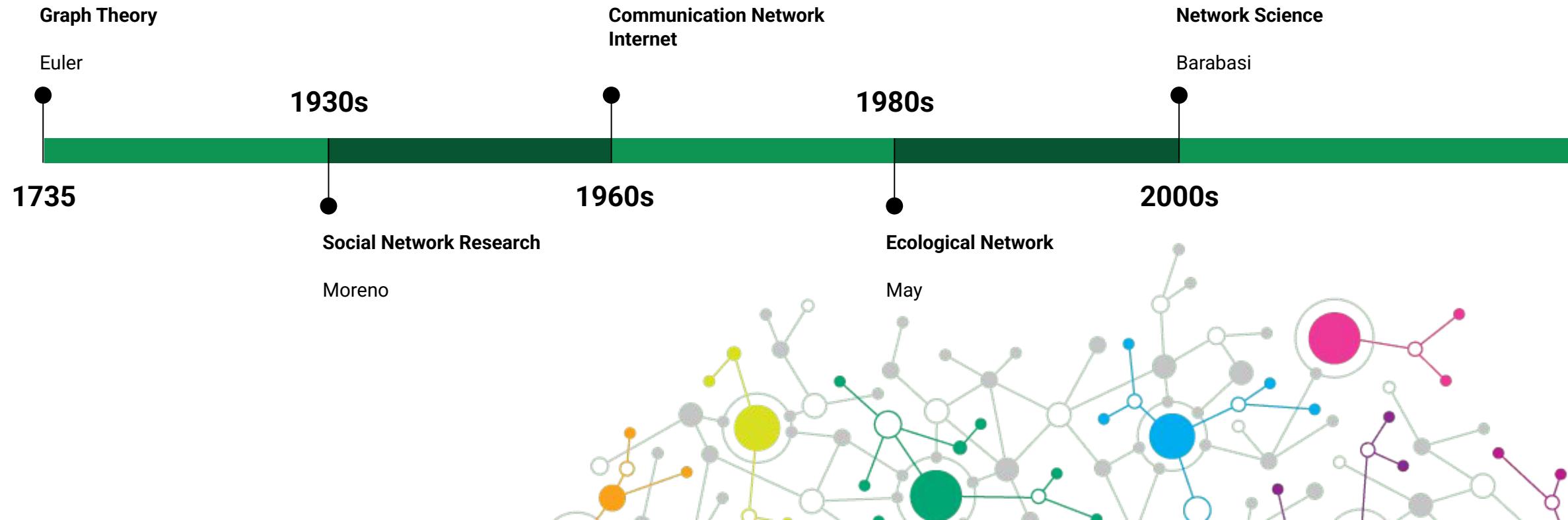
statista

Social Media Totals



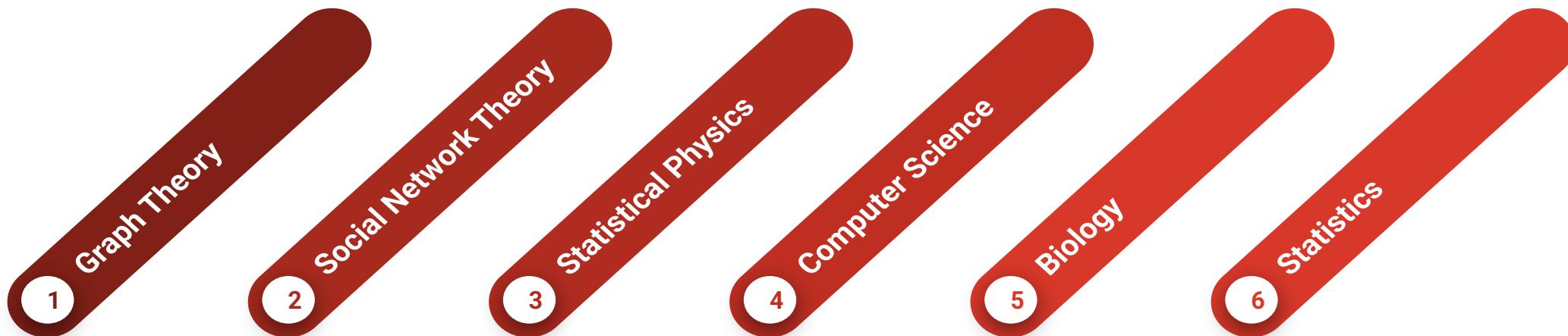
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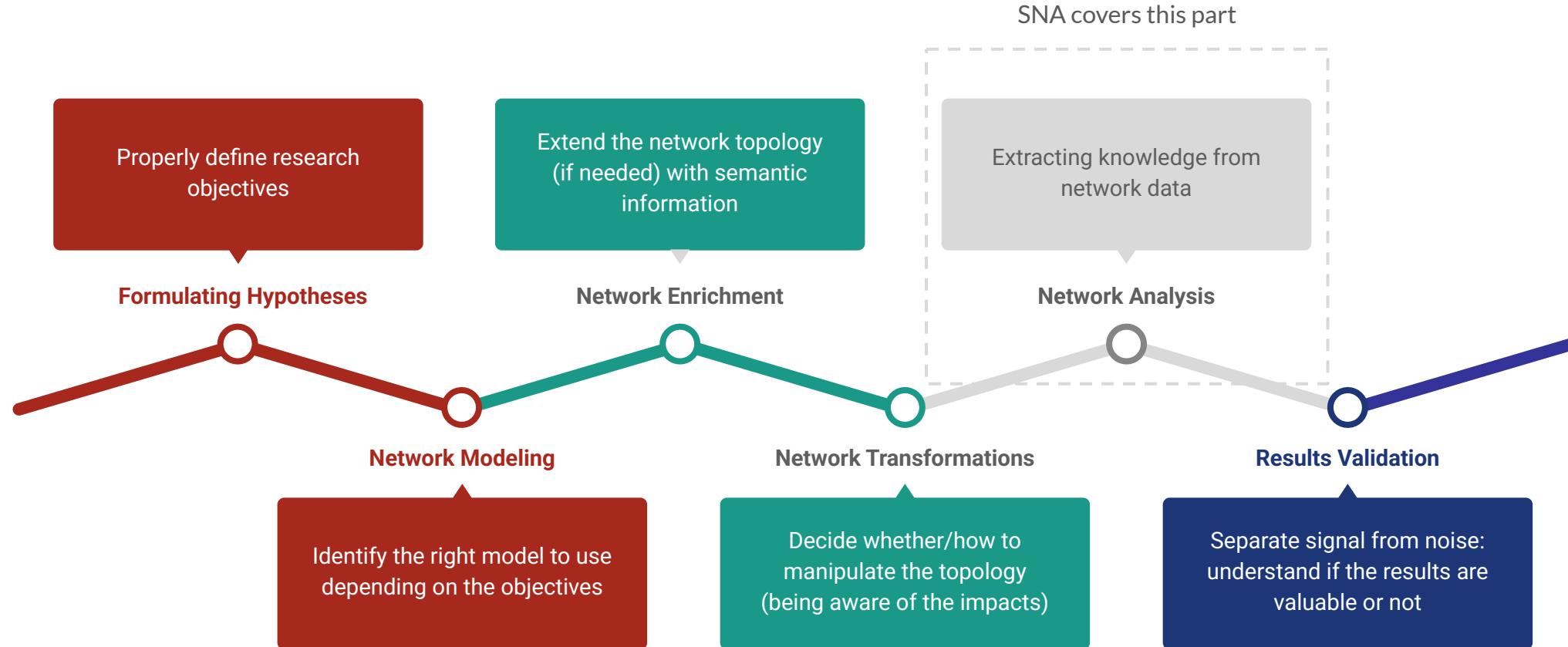
History of Network Analysis



The Tools of

Modern Network Theory







patrick.terrematte@ufrn.br

 **Discord** patrickterrematte



Prof. Dr. Patrick Terrematte