

Computational Systems Biology

Master Bioinformatica

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Course Presentation

Goals

- Learn the theory of biological networks topologies and analysis, but emphasizing the ***practical aspects***
- Be able to conduct systems biology modeling and analysis ***research projects*** in real life
- Learn the most used and ***advanced*** computational tools
- Known the state of the art of systems biology
- Be able to work in bioinformatic ***workgroups*** to conduct a research project
- Learn the best practices and general tools in *bioinformatic* research projects
- Encourage ***self-education***

Course Presentation

Contents

- ~15 classes
 - Biological networks overview: topology properties and centralities
 - Network modeling, visualization and analysis I (Cytoscape) **
 - Network modeling, visualization and analysis II (R and Python) **
 - *Advanced* graph theory **
 - Biological networks (regulatory, PPI, correlation, motifs, analysis and algorithms, ...)
 - Biological networks data, databases and formats
 - Network clustering and inference **
 - Biological networks dynamics
 - Seminars: analysis, networks evolution, metabolomic, metagenomics, ... (5 days)
 - Research project (1 day)
 - Invited speakers (1 day) **
- ** will be given by invited speakers

Course Presentation

Evaluation

- Evaluation
 - Exercises during the course (20%)
 - Presentation and questions (30%)
 - Groups of two people, 30 min presentation + 15 min questions
 - All people not presenting **must** prepare and ask a question
 - Research work: poster and paper (50%)
 - Groups of 4-5 people must carry out a research project. Scientific poster must be presented and a research paper written. Bioinformatic Journal template will be used. Each paper will be reviewed by 2 teachers.
- Exercises and workgroups will make use of *GitHub*
- No exam planned, all exercises and presentations are **mandatory**

Introduction

Definition (from *Wikipedia*)

- **Systems biology** is an emerging approach applied to biomedical and biological scientific research.
- Systems biology is a biology-based inter-disciplinary field of study that focuses on complex interactions within biological systems, using a more ***holistic*** perspective (holism instead of the more traditional reductionism) approach to biological and biomedical research.
- One of the outreaching aims of systems biology is to model and ***discover*** emergent properties, properties of cells, tissues and organisms
- Involve *biological networks* and makes an intensive use of *computational* methods
- New paradigm: from ***Functional Genomics*** to ***Systems biology***

Introduction

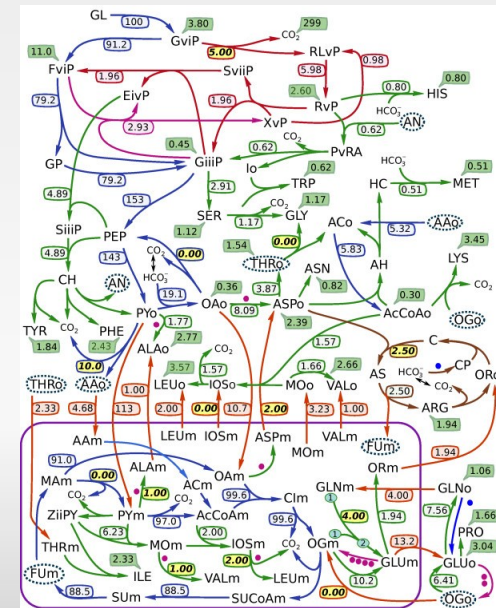
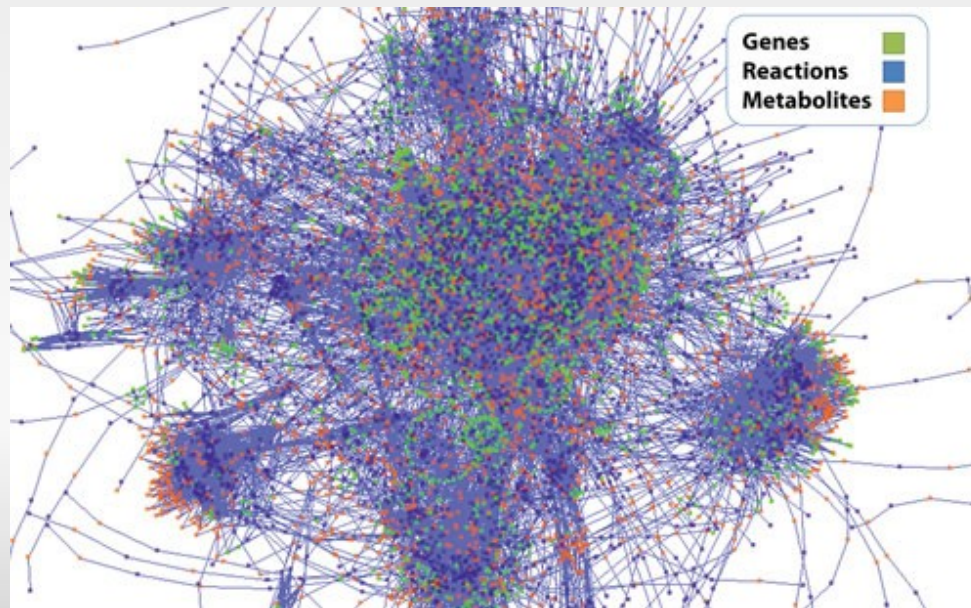
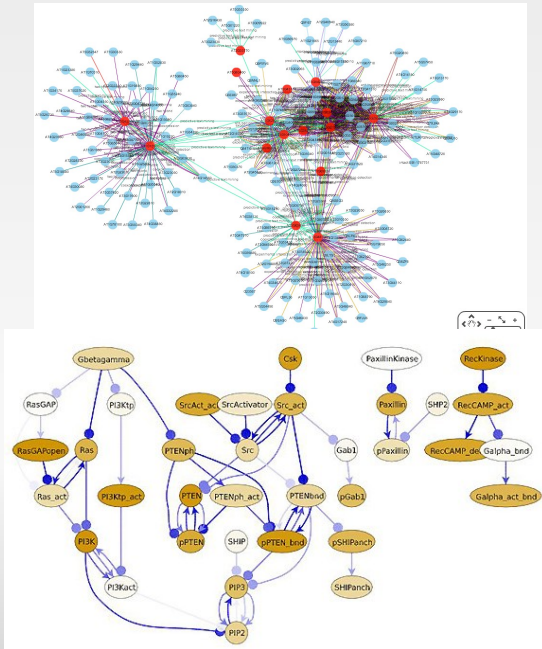
Holism vs Reductionism

- **Holism**, from *holos*, a Greek word meaning all, *whole*, *entire*, *total*
 - Represent the idea that natural systems (physical, biological, social, economic, etc.) and their properties should be viewed as wholes, not as collections of parts
 - Includes the view that systems function as wholes and that their functioning cannot be fully understood solely in terms of their component parts
- **Reductionism**, can be viewed as the opposite of *holism*
 - In science says that a complex system can be explained by reduction to its fundamental parts
- Open discussion? TO-DO read Brenner paper at GitHub repository

Introduction

Biological networks

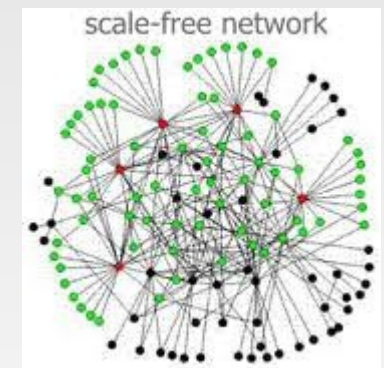
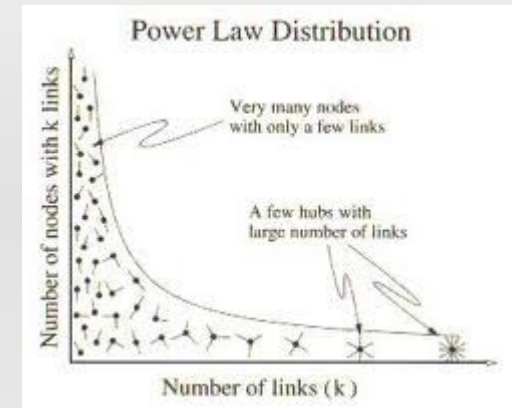
- Network types: protein-protein interaction, gene regulatory, signaling, metabolomic, correlation, ...
- Help us to understand how the different molecules interact each other and are regulated



Introduction

Network topologies and properties

- Topologies
 - Random networks
 - Scale-free networks
 - Hierarchical networks
- Properties
 - Small world
 - Degree distribution
 - Clustering coefficient
 - Betweenness centrality
- TO-DO: to read Barabasi 2004 review at [GitHub](#)



Introduction

Network models

- Network models
 - *Erdős-Rényi*: the most basic model of a random network. Binomial degree distribution. Reproduce small world but fails to local clustering coefficient
 - *Watts-Strogatz*: Good local structure and small average path length
 - *Barabási-Albert*: generate a scale-free degree distribution
- Additional properties of complex networks
 - Structural robustness and attack tolerance
 - Modularity and community structures
 - Subgraphs and motifs

Biological databases and formats

- Databases: manually curated vs computational predicted
 - Reactome
 - IntAct
 - String
 - BioCyc
 - ...
- Formats
 - BioPax
 - PSI-MI
 - SBML
 - Sif
 - ...

Computational tools

- Cytoscape
- R
- Python
- ...

Git and GitHub

- Git, the best SCM available
 - Allows sharing code
 - Tracking changes
- GitHub
 - A public and open git repository