Interaction Networks

Several Bio Networks

- Biochemical Pathways: sequences of chemical reactions involved in biological functions
- Metabolic pathways: sequence of chemical reactions, each reaction is catalyzed by a specific enzyme, and the product is the substrate for the next one
 - Catabolic pathways: disassembly of complex molecules to form simpler products (energy released) e.g. glycolysis
 - Anabolic pathways: synthesis of complex compounds out of simpler ones (energy required)
- (Gene) Regulatory Networks: describe the interaction between transcription factor proteins and genes that they regulate
- Signal Transduction
- "Interactome": all biomolecular interactions occurring in the cell under given conditions

Protein-Protein Interaction Networks

- We do not cover how networks are experimentally discovered and studied
- PP interactions can be studied in the first place by accounting for pairwise "interaction" or "binding"
- PP interactions among a given set of proteins can be represented by a graph, where vertexes represent specific proteins and edges represent "binding"
- PP networks can be analyzed by investigating the features of the corresponding graph

Topological Indexes of a Graph (I)

- Degree of a vertex: # of its connection edges
- Degree distribution: $p(k) = (1/N) ||\{v_i|deg(v_i)=k\}||$
- Poissonian p(k) in random graphs $p(k,\lambda)=(\lambda^k e^{-\lambda})/k!$
- In so-called scale-free networks, for k>>1, $p(k) \propto k^{-\gamma}$, $\gamma \in \Re^+$, usually $2 < \gamma < 3$
- Scale-free networks: ratio between the # of highly connected nodes and # of low connected ones does not depend on the graph size
- Scale-free -> small world phenomenon

Topological Indexes of a Graph (II)

- *Clique*: subgraph which is complete. The size of a clique is its number of vertices.
- Clustering coefficient C_i of a vertex v_i: how much the neighborhood of a vertex is far from being a clique
- $C_i = |Nb_i| / [k_i(k_i-1)/2]$ (undirected graph)
- Importance of *hubs*
 - Party hubs simultaneous interactions
 - Data hubs different times/locations

Data Structures for Graphs

- Adjacency list: for each vertex, store the list of neighbor vertexes
 - Cons: checking the presence of an edge, O(n)
- Adjacency matrix (n×n): entry m_{ij} is set to true if an edge exists between i and j.
 – Cons: storage requires O(n²)
- Incidence matrix (n×m): vertexes are labeled from 1 to n and edges fro 1 to m; entry b_{ij} is set to true if vertex i belongs to edge j.

Gene Regulatory Networks



Gene Regulatory Networks



Metabolic Networks

Kinetic Modeling of Cellular Processes Kinetic Modeling by ODE

Kinetic Modeling by Monte Carlo Approach



- Initialization
- Monte Carlo step
- Update
- Iterate

Integrated Networks



