2. Visual Analysis of Multivariate Biological Networks
Information Visualization (186.141)
TU Vienna, Austria
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2.1 Introduction

- Genomes: only 5% genes consisting of Exons and Introns
- RNA: Uracil instead of Thymine, single strands

2.1.1 Tasks of Bioinformatics

- Support of biologists within processing, analysis and interpretation of large data sets
- Approaches:
  - Biological data bases
  - Methods for comparison and function prediction of sequences
  - Function prediction of proteins
  - Locating of new correlations
  - Simulation of biological processes

2.1.2 Visualizations

- Visualizations of networks and related structures
  - Networks
  - RNA-secondary structure
  - Phylogenetic trees
- Visualizations of sequences
  - Sequence alignments
- Proteins
  - Structure prediction
  - Structure comparison
  - Protein dynamics

Correlations: Genome – Chromosome – Gene – DNA

DNA: Double helix with nucleotides from sugar, phosphate and four bases
(Adenin, Cytosin, Guanin, Thymin)

Proteins are built by amino acids
- 20 amino acids: coded by nucleotide triplets (Codons)
  - e.g. GCA, GCC, GCG → Alanin

Here, we will focus on these issues!
2.2.1 Motivation

There is a hierarchy of such biological networks

- Molecular Graphs
- Metabolic Networks
- Interaction Networks
- Regulatory Networks
- ...

Why is that important?

- Diseases can be explained in context of networks
  - Infection: a foreign network starts operating in our own network
  - Genetic defects: incorrect connectivity of an element

- Applications
  - Drug design, metabolic engineering, …
2.2.2 Metabolic Networks

- Paths: Sequence of reactions that provide all together for the translation of one substance into another one (pathways)
- One single reaction is defined by a catalyzing enzyme
- Example:
  \[
  \begin{align*}
  &\text{2-Phospho-D-glycerate} \\
  \rightarrow &\text{Phosphoenolpyruvate} \\
  \rightarrow &\text{Pyruvate} \\
  \rightarrow &\text{ATP} \\
  \rightarrow &\text{ADP} \\
  \rightarrow &\text{H}_2\text{O}
  \end{align*}
  \]
- As a whole, the paths build a so-called metabolic network (MN) \([\rightarrow \text{Graph}]

Limneus University
2.2.2 Metabolic Networks

Visualization of Simulation Data

[Video Leipzig & Linnaeus Univ., 2009]


2.2.2 Metabolic Networks

Interrelationships between network components

[Video Linnaeus Univ. & IPG Gatersleben, 2012]


http://sourceforge.net/projects/gliep/

2.2.3 Protein-Protein Interactions

Nodes are proteins and edges the interactions between them

Interactions between proteins are important for many biological functions

Example

- Signal Transduction: signals from the exterior of a cell are mediated to the inside of that cell by protein-protein interactions of the signaling molecules
- It plays a fundamental role in many biological processes and in many diseases

http://en.wikipedia.org/wiki/Protein-protein_interactions

2.2.4 Special Visualizations

Comparison of biochemical networks

[U. Brandes et al. Integrative Bioinformatics, 2004]
2.2.4 Special Visualizations

- **Visualization of Network Centralities**

2.3 Phylogenetic Trees

- **Problem**
  - Analysis of the development history of today’s species and their relations

- **Example:**

```
<table>
<thead>
<tr>
<th>hypothetical ancestors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Siamang</td>
</tr>
<tr>
<td>Gibbon</td>
</tr>
<tr>
<td>Orangutan</td>
</tr>
<tr>
<td>Gorilla</td>
</tr>
<tr>
<td>Human</td>
</tr>
<tr>
<td>Chimpanzee</td>
</tr>
</tbody>
</table>
```

2.3 Phylogenetic Trees

- **Objects**
  - Species, populations, DNA, proteins

- **Tree**

  - rooted
  - event. weighted
  - unrooted

- There are two methods for the determination of the root
  - Outgroup method: with not-related objects
  - Hypothesis of a molecular clock: root has the same distance to all objects

2.3.1 Visualizations

- **Example tool:** PHYLODRAW
  - Presented by Choi et al., ‘00

2.3.1 Visualizations

- **Example tool:** TreeJuxtaposer
  - Presented by T. Murzner et al, SIGGRAPH ’03

- **Focus & Context**
  - “Guaranteed visibility”
  - Computing structural differences