BioEdge: a tool box for advanced analyses of biochemical networks

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The Challenges

- Integration of different types of networks : metabolic, regulatory, signal transduction
- Analyzing these networks provides valuable clues on the system level behavior
- Elaborated analyses
  - Involve solving complex combinatorial problems
  - Size of the network tends to be large
- Need for sophisticated computational methods and algorithms

The BioEdge tools

- Graph properties
- Path and subgraph finding
- Context Extraction
- Motif extraction
- Graph Matching

Research Context

- The BioMaze and TransMaze projects
- Representation, **Analysis** & Visualization of biochemical networks
- Interdisciplinary and interuniverity projects
- Funded by the Walloon Region, Belgium (2003-2008)

Research Approach

- The BioEdge underlying tools are mostly domain independent
- Analysis of large graphs
- Using standard (efficient) approaches
- Using the Contraint Programming and the Machine Learning frameworks

Implementation

- Java technology
- Initial tool box : Eclispe plugins in the BioMaze environment
- New implementation : **Cytoscape** plugins

References

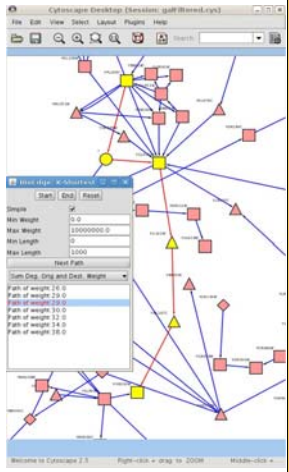
[1] V. Jiménez, A. Marzal. Computing the K Shortest Paths: A New Algorithm and an Experimental Comparison LNCS 1668, Springer Verlag, 1999

[2] Jérôme Callut. First Passage Times Dynamics in Markov Models with Applications to HMM Induction, Sequence Classification and Graph Mining. Ph.D Thesis, UCL/INGI, October 2007

Path and Subgraph Finding

Two complementary approaches

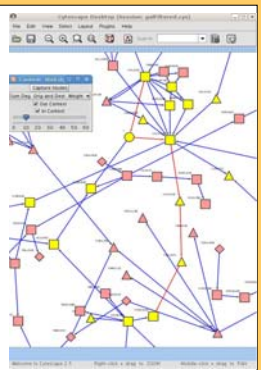
- **K-shortest paths**
  - Implementation of a classical efficient k-shortest paths finding algorithm [1]
  - Various weight policies
  - Directed and undirected networks
  - Can be combined with various filters (path without loop, mutually exclusive nodes, length of the path, …)
- **Constrained path finding**
  - Based on constraint programming
  - Allow sophisticated subgraph extractions



Context Extraction

Two complementary approaches

- **Neighbourhood of a subgraph**
  - Given a path / subgraph, visualize its context
  - Extract the neighbours of the subgraph in its context
  - Specify the width of the context



- **Extraction of a relevant subgraph**
  - Given a set of nodes
  - Extract a subgraph that best explains the relation between these nodes
  - Novel method based on graph data mining [2]
  - Specify the level of relevance