

Literary Research on Graph Theory

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Mathigon Graph Theory

http://world.mathigon.org/Graph_Theory

- Basic overview of graph theory, illustrating the same main points as say, Wikipedia does
- Outlines the basics and initial word problems of Graph Theory (7 bridges of Königsberg, Traveling Salesman, Four color theorem, etc.)
- Also brought up the different usages of networks
- Only new concept discussed here was Euler's Formula which calculates how many "faces" there are in a network ($\text{faces} + \text{vertices} = \text{edges} + 1$)
- Disregarded as calculating the faces seems unimportant for the networks we're making

An efficient graph theory-based method to identify every minimal reaction set in a metabolic network

Sudhakar Jonnalagadda and Rajagopalan Srinivasan

- This article was exploring the metabolic networks for microorganisms breaking down different chemicals and their bioprocesses
- They are trying to streamline the networks into one minimal reaction set and taking out redundant pathways.
- Used a program called MILP (Mixed-Integer Linear Programming) to find the minimal reaction set by analyzing the optimization parameters of flux distribution, metabolic capabilities, etc.
- Their networks had far more flux and flux dependency (not linear) than ours and was set aside as our minimal reactions are manually found by deletion of strains

Feizi, S., Marbach, D., Médard, M., & Kellis, M. (2013). Network deconvolution as a general method to distinguish direct dependencies in networks. *Nature biotechnology*, 31(8), 726-733.

- This article was dealing more with very large networks that have long connections and nonlinear indirect flows.
- Here, they used “message-passing algorithms” and “variations of granger causality” to try capture the most dynamic relationships and wrote an algorithm to deconvolute the networks
- Their algorithm solved inverse problems of transitive closure by decomposition of eigenvectors and eigenvalues
- Mainly appeared to be taking out feed-forward edges (Only displaying $A \rightarrow B \rightarrow C$ instead of both $A \rightarrow B \rightarrow C$ and $A \rightarrow C$)

Pavlopoulos, G. A., Secrier, M., Moschopoulos, C. N., Soldatos, T. G., Kossida, S., Aerts, J., ... & Bagos, P. G. (2011). Using graph theory to analyze biological networks. BioData mining, 4(10), 1-27.

- This article mainly focused on protein-protein interaction networks but do discuss gene regulatory networks (GRNs) as well
- When discussing graph properties, the path length, diameter, and simple paths of all of these networks came into play
- We decided the betweenness centrality and degree distribution are the two most relevant subjects on this paper and that writing MATLAB script to try to try to automatically generate info from this are our next steps.

Gostner, R., Baldacci, B., Morine, M. J., & Priami, C. (2014). Graphical modeling tools for systems biology.

- This article is a review of computational tools that have the main graphical formalisms in modeling biological systems. The review analyzes the elements present in different systems, through a lens of looking at the usability of the computational tools.
- Different tools were then ranked based off of more specific criteria under the categories of modeling, editing, interoperability and visualization
- Packages for Matlab weren't looked at, but there are a couple visualization programs that might prove useful for GRNsight (see figure 2 in paper for capabilities)

Hsiao, Y. T., & Lee, W. P. (2014). A Knowledge-Guided Approach for Inferring Gene Regulatory Networks. In *Intelligent Computing in Bioinformatics* (pp. 186-192). Springer International Publishing.

- Paper discusses how reverse engineering can be used to reconstruct gene regulatory networks, similar to what we are focusing on
- Focuses on optimizing the accuracy of inferred behaviors of the network, and on designating valid biological topologies for target networks. They present an integrative modeling framework to meet these two criteria.
- The framework combines inputs based in the literature and knowledge and inputs based on the data.
- Through experimentation on their algorithms, the authors were able to validate their approach
- In testing their proposed approach and method, the authors used a 5-node network that was to be used because the artificial network is both popular and small, which fits their space limitation. This may be good for us as it has been suggested that we focus on smaller gene regulatory networks with fewer nodes in our testing

Murphy, K. (2001). The bayes net toolbox for matlab. *Computing science and statistics*, 33(2), 1024-1034.

- Bayes net toolbox is an open-source matlab package for graphical models for a variety of probabilities for the nodes, and for static or dynamic graphs
- Paper covers a variety of features of the toolbox, mostly focusing on inference and probability in the background of what the toolbox can do.
- Paper offers good comparison figure (Figure 2, Section 7) of different toolboxes available in MATLAB for implementing code that focuses on graph functions. Figure is most likely dated though, as the paper was published in 2001, but good starting place for finding features we want to include in GRNmap