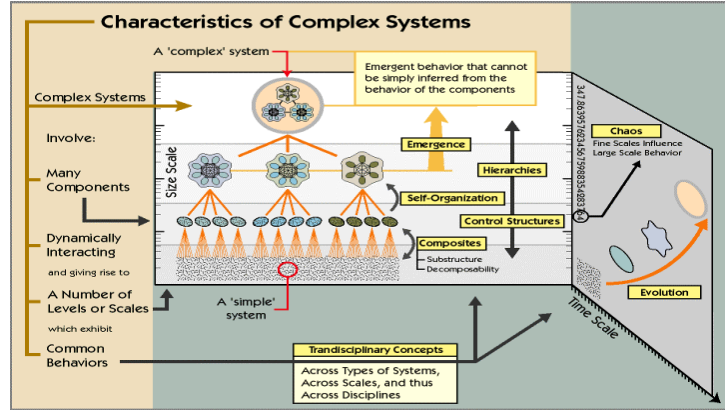


BIOINFORMATICS AND COMPLEXITY THEORY– WHY BOTHER?

TARYNN M. WITTEN

DIRECTOR, RESEARCH AND DEVELOPMENT,
CENTER FOR THE STUDY OF BIOLOGICAL COMPLEXITY

When we think of bioinformatics, we typically think of gene sequences, databases, alignment and searching, and string pattern searching or pattern matching algorithms. More recently, complexity theorists have entered the game, bringing with them a larger view of the problem. No longer is it sufficient just to examine the lower-level



problems that previously engaged researchers. Now we must begin to examine problems at a larger scale. Given a set of genetic knockouts, how do we construct a metabolic pathway/metabolic network?

Suddenly, we are faced with the problem of simulating such a network in a larger environment that may incorporate multiple cellular interactions, organ and organ system interactions, and socio-cultural - environmental interactions. It may be critical to incorporate GIS techniques to examine virus spreading or the development of malaria, schistosomiasis, or SARS. Incorporating levels of behavioral dynamics requires not only layers of biomedical understanding, but also computational skills that

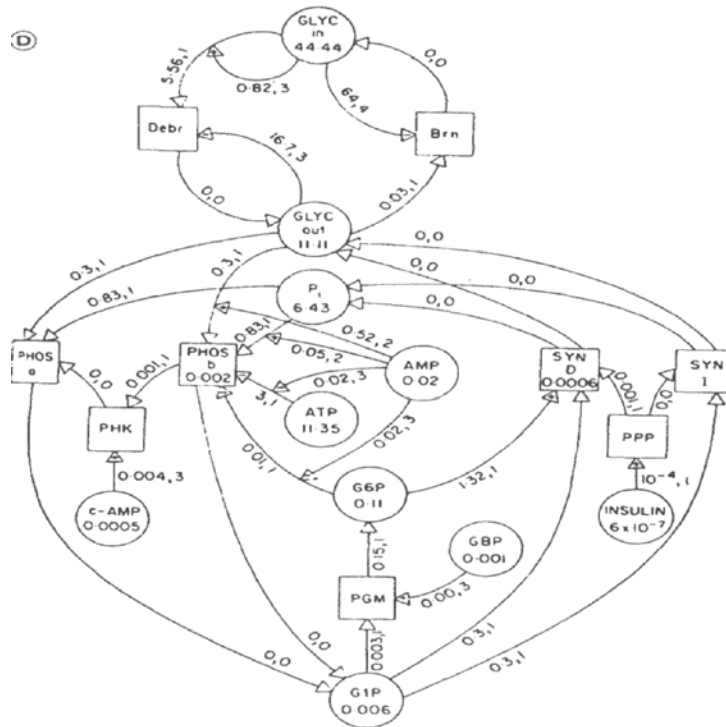


Fig. 1. (a) An illustration of an undirected graph (network). Here, we consider the "coarsest" possible description; namely, that the elements are connected. The dependence (direction) of the connection is ignored. (b) A sample directed graph created from the network illustrated in (a). (c) An illustration of the nodal representation of (b). (d) A graph representation of a model for glycogenolysis. Reproduced by permission of the authors, Kohn and Letzkus [3].

involve the use of high performance computing environments, advanced programming skills, sophisticated mathematical tools and techniques, and a unique worldview that can see the larger problem. It is this set of tools that complexity theory brings to these larger scale research efforts.