

## Complex Networked Systems: Foundations and Implications

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**Keywords:** complex networks, structural complexity, dynamics.

In 1999 Barabási and Albert<sup>1</sup> showed that real networks of very different kinds had a common signature, a power law degree distribution, and proposed a simple model to explain it. This discovery has been confirmed in fields as diverse as biology (metabolites, neurons, cortical areas, protein-protein interactions), technology (Internet, WWW, transportation, power grid), ecology (food webs), social sciences (collaboration, scientific citations, virtual social networks, e-mail), economy (world trade, patents), linguistics (words co-occurrence, free association), etc. The existence of “universal” properties in these networks, together with the increasing availability of real data, has promoted complex networks to be one of the main research topics during the last decade<sup>2,3</sup>.

Complex networks (or graphs) appear every time you have objects or entities (nodes), and relationships between them (edges or links). For instance, in social sciences the nodes are usually persons and the edges may represent friendship, collaboration or trust, while in biology the nodes could be metabolites, proteins, genes, neurons or species, and the edges account for interactions, synapses or food. Sometimes graphs are artificially built for the analysis of systems which do not have nodes and edges. For example, time series can be discretized in a finite number of states (the nodes), and the transitions between them define the links. Another example, now in chemistry, is the network of the potential energy landscape<sup>4</sup>, where the basins of attraction are connected by the transition states. In Fig. 1 we show an example of a dolphins' social network.

The term “complex” is used for two reasons: to distinguish these real networks from completely regular (lattices) and completely random graphs; and to include them in the class of “complex systems”. In a few words, a complex system is any system in which simple constituents, with simple dynamics, yield emergent unexpected phenomena, such as phase transitions or collective behaviors. Complex networks satisfy this definition both from the structural (topological) and the dynamical points of view.

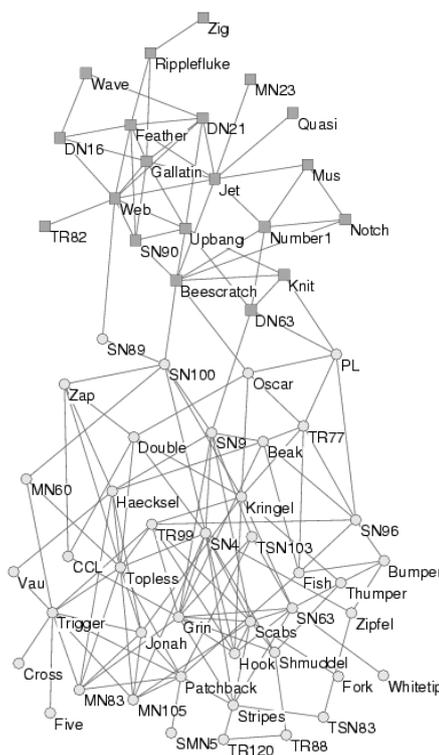


Fig. 1 – Dolphins social network<sup>10</sup>. The nodes correspond to 62 bottlenose dolphins observed in the period from 1994 to 2001, and the links represent the associations between dolphin pairs occurring more often than expected by chance.

There are different classes of complex networks, depending on the structure and the information attached to nodes and links. A network could be directed or undirected (edges with or without direction), weighted or unweighted (edges with or without an assigned real value), bipartite (nodes of two classes and edges only between nodes of different class), multilayered (nodes of different classes), colored edges (edges of different classes), hypergraphs (edges connecting more than two nodes at the same time), etc.

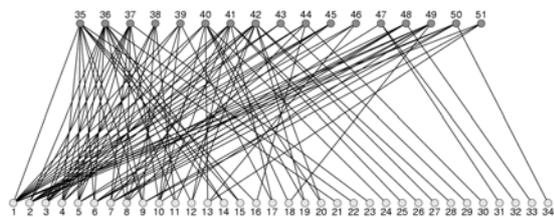


Fig. 2 – Bipartite network of solvents: chemicals in the bottom and industrial applications in the top.

Among the recurrent structural properties found in many complex networks we could mention the following ones: power law degree distributions<sup>1</sup>; small-world property<sup>5</sup>; community structure<sup>6,7</sup>; high transitivity<sup>5</sup>; assortativity<sup>8</sup>. Some of these properties are trivial for certain networks, but may be quite surprising for others. For instance, in social science, the transitivity may be stated by the sentence “the friends of my friends are also my friends”, which is easily accepted. However, why should a metabolic network exhibit high transitivity and a community structure? Which are their evolutionary and functional explanations? This is one of the key points in complex network research: the uncovering of the relationships between structure and function.

The analysis of the topology of complex networks allows the quantification of important properties of nodes and links such as their centrality, the role played by nodes in their communities, the existence of erroneous and missing links, the robustness of the network against failures or attacks, or the existence of rich clubs. As an important example, Google’s PageRank algorithm<sup>9</sup> to sort web pages according to their relevance is just one of the many centrality measures defined for complex networks.

The dynamics which take place on top of complex networks inherit the complexity of the underlying structure, giving rise to interesting phenomena. The diversity of dynamics which have been studied is large: diffusion, epidemic spreading, rumor and opinion spreading, synchronization, random walks, routing, evolutionary games, percolation, etc. Many of them undergo second order (and even, first order) phase transitions, local heterogeneities, and other kinds of global behaviors which are difficult to anticipate from their apparent simple rules.

Complex networks appear easily in all kind of knowledge areas, and Chemistry (and Green Chemistry as a particular case) is not an exception. However, little effort has been dedicated to this end, and no public networks are available. The easiest set-up would be a network where the nodes are chemicals and the links represent any kind of relationship between them, e.g. structural or functional similitude. An interesting case is the network in which we have two types of nodes,

chemicals and industrial applications, and the links connect each chemical with its known applications. In Fig. 2 we show this bipartite network for a database of solvents. It is easy to realize that many chemicals have few edges, while few of them have many links, which is what you find in power law degree distributions.

We do not know what results could be obtained from the application of complex network concepts, theory and algorithms to Green Chemistry, but the large degree of success in other areas point to the need of further research.

### Acknowledgements

This work has been partially supported by MINECO through Grant No. FIS2012-38266.

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