Complex Structures and Dynamics

Applications to Chemistry, Biology, Social Science and Economics

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Abstract

Definition of basic structures and events. The difference between events and structures is a matter of modeling. Structures are defined as permanent, their ontology is that of classes or types with certain characteristics. Events on the other hand are singularities inside the time arrow which as the word suggests is assumed to have a direction and furthermore assumed to be continuous.

Basic remarks

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- Also the relations between types are in most models fixed. But it makes sense sometimes to let either types or relations change over time, typically triggered by an event. Evolutionary models will be an example.
- Relations between types can always be interpreted as memberships of the types. Memberships can be *symmetric* or *asymmetric*.

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- The basic ontology of a type is that it can either exist or not exist. This is a basic modeling choice. The modeler creates her or his own interpretation of reality. In more complex models there will be additional structure. One of the first steps usually taken is that types become populated, i.e. there is a number attached to the type. In basic models this number is an integer, but it can become a real number by scaling.

Graph Theory as a Special Case

A graph G (or network) is a set of points or nodes (always called vertices in graph theory) V in space which are interconnected by a set E of lines or links (always called edges in graph theory), i.e. $G = (V, E)$.

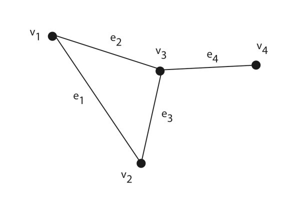

Figure: Example of an undirected graph G.

Here $G = (\{v_1, v_2.v_3, v_4\}, \{e_1, e_2, e_3, e_4\})$. Let $|S|$ denote the number of elements of a set S. If both $|V| < \infty$ and $|E| < \infty$ then the graph G is called finite. For any edge e joining the vertices v_i and v_j we set $e = (v_i, v_j)$. Because so far the vertices have no direction, we have also $e = (v_j, v_i)$. In this case G is called *undirected*.

An undirected graph describes a binary relationship between a set of vertices.

- If an edge e has v as en end-point, then e is called incident with v.

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- Two edges are adjacent if they have a common end-point.

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Let $k := d(v)$ and $P(k)$ be the degree frequency (which can be interpreted as a degree probability distribution) in different types of graphs.

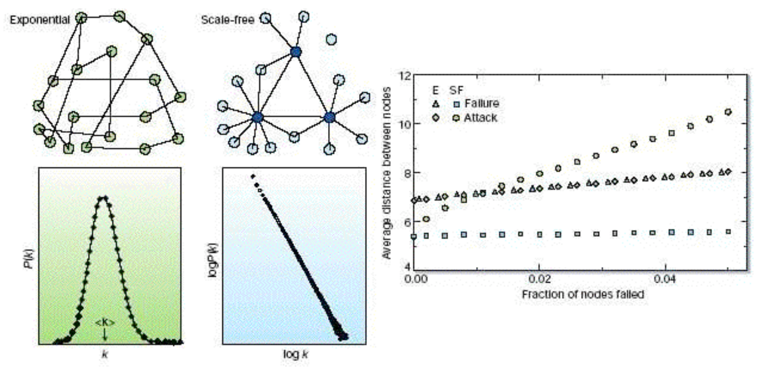
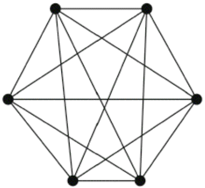


Figure: Examples of different types of degree distributions.

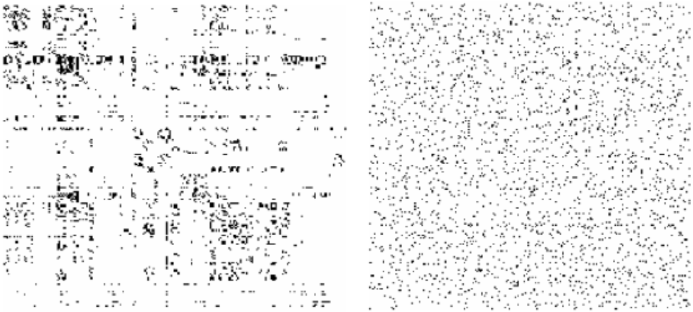
Algebraic Graph Theory

Graphs can be analysed algebraically (a very fruitful concept!) by introducing adjacency and incidence matrices. In a graph $G = (V, E)$ define an $(n \times n)$ symmetric matrix $A = (a_{ij})$ by $a_{ij} = 1$ if $(v_i, v_j) \in E$ and zero otherwise. This adjacency matrix encodes all information on G. Powers of A can be used to calculate the number of paths between vertices. The coefficients of the characteristic polynomial of A encode information on the number of edges, triangles (the number of times the complete subgraph K_3 wth 3 vertices occurs in G) etc.



$$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

The adjacency matrix can even be analysed visually: Comparison of a random graph with the C. elegans neuronal network.

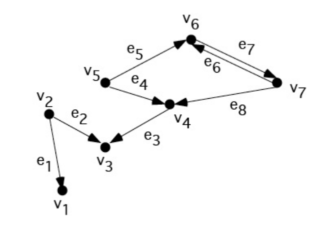


C. Elegans network

Random Network

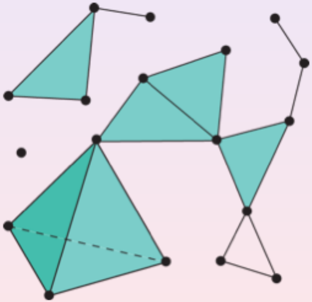
Directed Graphs

After giving the graph $G = (V, E)$ an *orientation* (of the edges) the result is a directed graph $\vec{G}$. Instead of a binary relationship such a graph can model hierachical relations, like 'x is more dominant than y', 'x is influencing y', 'x regulates y', etc. The adjacency matrix A of $\vec{G}$ becomes in general non-symmetric. We can define an $(n \times m)$ incidence matrix $D = (d_{ij})$ by $d_{ij} = +1$ if v_i is the positive end of e_j, $d_{ij} = -1$ if v_i is the negative end of e_j, and zero otherwise. The incidence matrix D resulting from giving an arbitrary orientation to G has rank $n - c$, where c is the number of components of G.



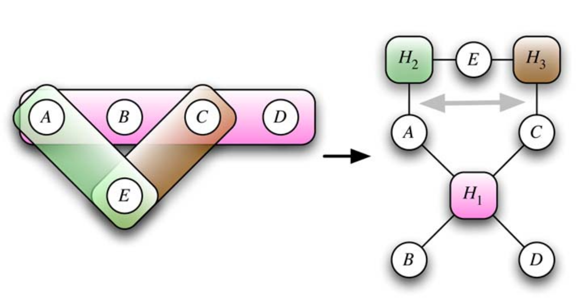
Generalised Structures: Simplicial Complexes

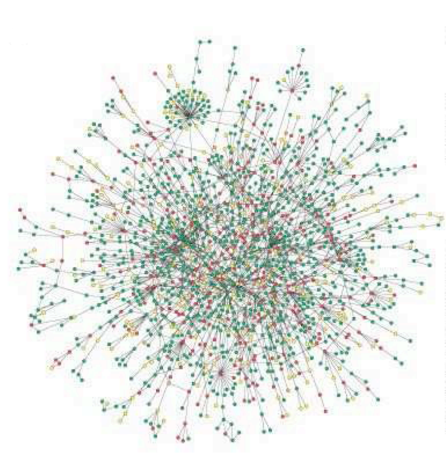
A (realization of a) simplicial complex can be interpreted as a generalization of a graph going beyond binary structures.



Generalised Structures: Hypergraphs

A (realization of a) hypergraph can again be interpreted as a generalization of a graph going beyond binary structures. But one can always restrict to graph theory: hypergraphs are equivalent to bipartite graphs. One can also see that hypergraphs are more general than simplicial complexes.





The first illustration of the yeast proteome network. Due to evolution this is in reality a growing network. It makes sense to introduce weights on this graph. For this additional measurements are necessary, for example protein size and binding affinities.

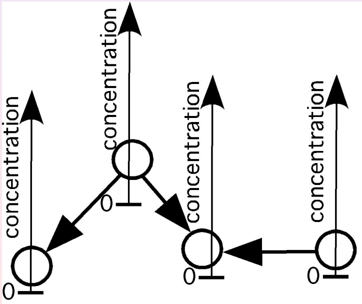
Weighted Graphs

The next mathematical possibility is to attach state spaces to the (static or evolving) graph, either to the vertices or to the edges. Let X be a finite set (i.e. X is either the set of vertices V or edges E) and $f : X \to K$ with $K = \mathbb{N}, \mathbb{R}, \mathbb{C}$. Usually the set of all such functions f form a vector space, i.e. the length of roads (the traveling salesman) usually adds up etc. But this depends on the model. The general idea of introducing state spaces is to attach numerical values to the relationships, or to make these relationships depending on some quantitative measure of the node (like size, richness, status etc.)

Generalisation: Vector-valued or function state spaces defined on K.
Data: ... (much more difficult, quantification of relationships)

Weighted Graphs as Networks with State Spaces

Weighted graphs are best interpreted as structures on which state spaces are defined. The next step then will be to assign a law or mathematical equation which is updating the state of the system in the combined state space, which is the Cartesian product of all individual state spaces.



Final Remarks

- The higher the dimension of the total state space the higher the degrees of freedom of the system, the more difficult to analyze the model mathematically (in general, but this depends on the 'law of motion' ascribed to the state space updates).

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- The more degrees of freedom the more data are needed to 'check' the model. Every model is a scientific hypothesis which according to Popper must be seeked to be falsified (a negative attitude is therefore scientific!)
- This also means every model in complex systems and elsewhere has an information theoretic aspect.