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ON THE ABC OF GRAPH APPLICATIONS (*)

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A is for ANTHROPOLOGY.
Claude Levi-Strauss does agree,
That all should read Hage & Harary
Who (alas) does not drive a Ferrari.

B is for BIOLOGY.
As everyone can plainly see
Animals are there and here
With billions more due every year.

C is for CHEMISTRY.
With and sans stability,
There are so many kinds
Which attract Nobel minds.

FOR EVERY FIELD
WHICH HAS SOME STRUCTURE
GRAPH MODELS YIELD
MATERIAL FOR A LECTURE!

1. What are mathematical models?

There are many independent discoveries in mathematics (as well as in all other sciences and in the social sciences). Indeed it is very often the case that two or more authors (or in these times of ever-increasing collaboration in research [15], more likely two or more sets of authors) will work on the same problem at about the

(*) Dedicated to my colleagues with whom books are being written on applications of graph theory to their fields: Per Hage, Anthropologist; Paul Mezey, Chemist; Hong-Sen Yan, Mechanical Engineer.

same time, and will publish the same result in different journals. Several examples of this phenomenon are given in [13].

In fact, some of the ideas in this section on mathematical models which is based on [12], have occurred to others.

Given a problem area in the real world which (implicitly or explicitly) involves sets an operation on sets, it is necessary, in order to make progress, to abstract the problem to a mathematical formulation. This abstract statement has been called a *mathematical model* for the real problem. The applied mathematician who is interested in this real scientific problem then directs his research activities to the purely mathematical statement. If he succeeds beyond the descriptive level, he will have found and proved one or more theorems.

If one had to specify a difference between mathematics and all other subjects, the answer should be that *only mathematics has theorems.* If a research article in a journal devoted to biology or chemistry or physics or economics or psychology or computer science or etc. contains a theorem, then there is a mathematical model involved and the theorem is a result in this branch of mathematics.

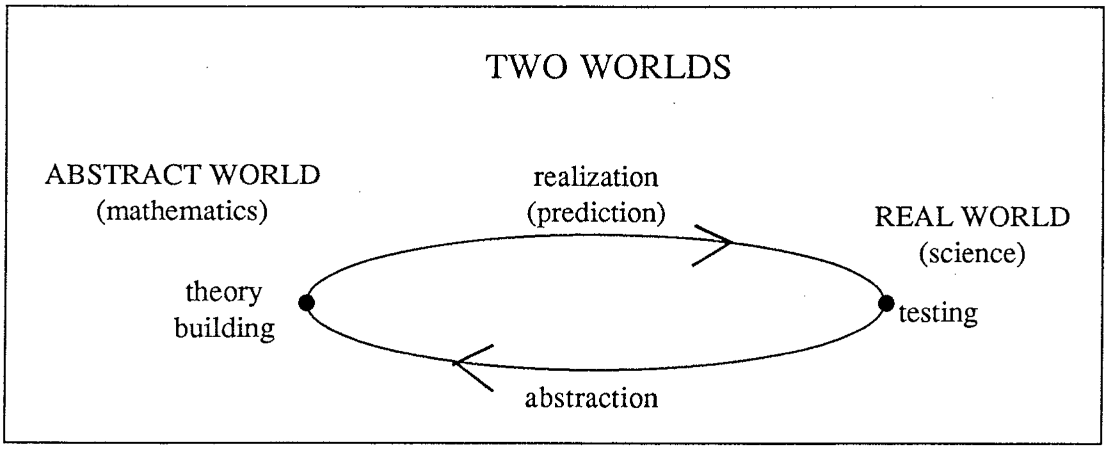

Figure 1 - Simple paradigm for mathematical models.

In Figure 1, a simple paradigm for mathematical modeling is displayed. The real world of science is on the right; the abstract world of mathematics on the left. Not surprisingly, the process of going from right to left is called *abstraction*, and that of going from left to right is *realization* which generally constitutes a prediction.

The prediction is tested and if it works, the mathematical model is retained; if not it is either discarded or modified.

In a more complex paradigm as in [12], which is useful for further clarification of the processes in mathematical modeling, each of the two worlds is again bifurcated into the high and low levels. The lower level on the left involves axiomatics and the foundations of mathematics and logic. The lower right contains the basic scientific laws of the subject. The process of developing theories may be depicted by an arc (on the left or right) oriented upward from the lower level to the upper level; it is called *derivation*. The reverse process has been called *selection*.

Our purpose is to indicate some mathematical models which have been applied successfully to anthropology, biology and chemistry, where the mathematics involved is restricted to graph theory.

2. Graph. Models in anthropology.

There is just one known example [6] of a paper authored by an anthropologist, published in a mathematics journal (with high standards). The phrase «some genuine models» in the title of that paper indicates that the graph theoretic concepts and results actually explain, clarify, and quantify the observed anthropological phenomena. (Alas there are too many papers in the literature of the social sciences, and indeed some in the physical and biological sciences as well as computer science, which claim to present mathematical models that do not, in fact, stand up to empirical verification. Such models, in words of one syllable, do not work. Hence they should be discarded).

The graph models for anthropology are denoted by A1, A2, etc.

A1. Trade.

Consider the graph $G = (V, E)$ where the node set V is the set of inhabited Marshall Islands in the Pacific Ocean, and the edge set E is determined by the trade routes between pairs of islands. Empirically, this graph G is a tree with one central node. This central island acquired the most power during the passage of time.

A2. Gift Giving.

In the set V of islands in the Pacific known as the «kula ring», there exists an established custom of presenting gifts from one island to other nearby islands, each year. The name of this island group comes from the fact that their geographic locations somewhat resemble a cycle shaped polygon.

Annually, arm bands are given in a clockwise orientation while rings and necklaces are gifts given in a conterclockwise direction. In a paper by Hage, Harary and James cited in [7], it was shown that the equiprobable Markov chain model on the digraph D of the kula ring yields a close approximation the actual distribution of the gifts among the various islands.

A3. Wife-Giving.

In small groups of nearby islands, in order to avoid the disasters of inbreeding, it has become the custom for the teen-age girls of one island to be sent to a neighboring island as wives. The greatest living anthropologist, Claude Levi-Strauss, found empirically that the two smallest directed cycles (shown in Figure 2) both occur in this way. Other small strongly connected digraphs also occur. This phenomenon was reported in our first book [5] on the uses of graphs in anthropology.

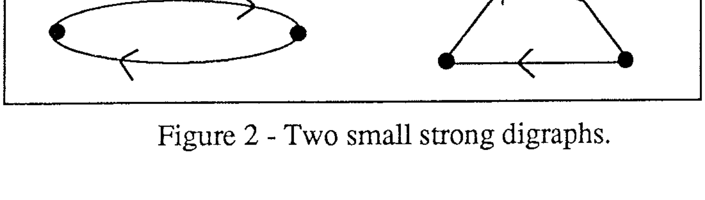

Figure 2 - Two small strong digraphs.

3. Graph models in biology.

Very often, mathematical models are deliberate oversimplifications of otherwise totally intractable real world phenomena. One such example was told to me by an anonymous biologist who studied the combinatorial structure of a tiny animal with a very small number of cells by assuming that each cell is a unit square and that the animal lies in the plane.

B1. Square Cell Animals.

The nine animals with at most four square cells are shown in Figure 3 together with intuitive names which have been assigned to them as suggested by their shapes.

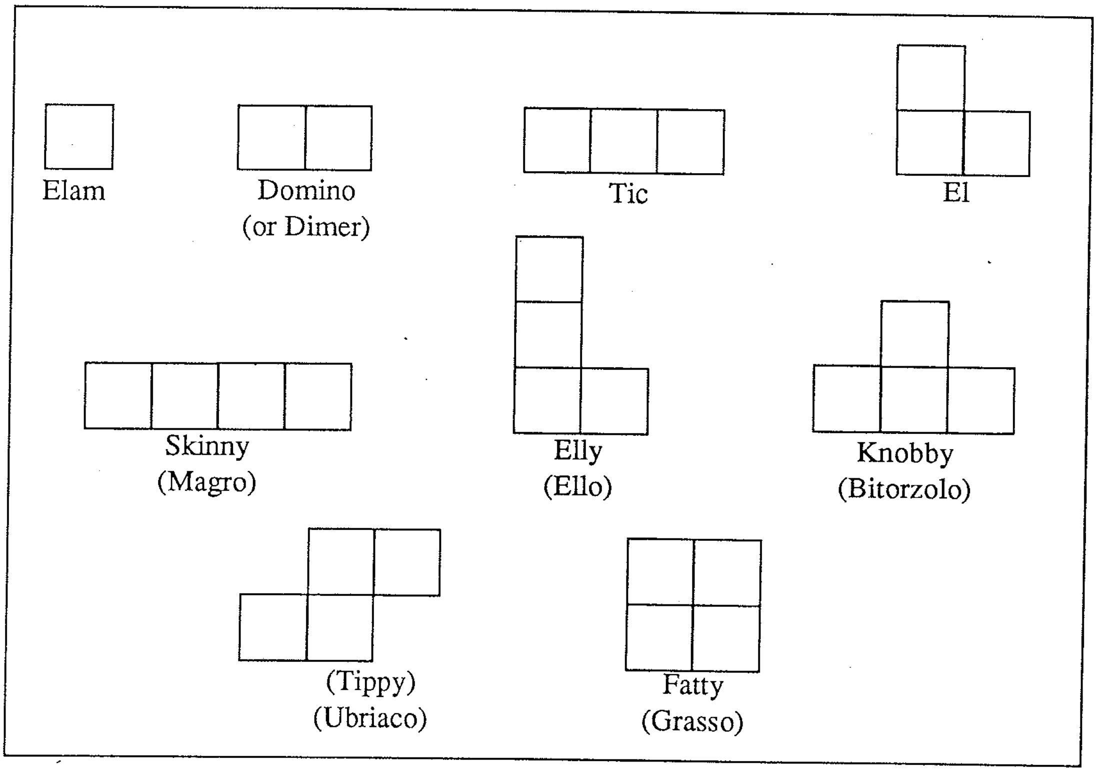

Figure 3 - The smallest square cell animals (with their names in English and Italian).

In my first article on animals [10], I asked for an explicit formula for the number of different animals with n cells. It appears that this problem is intractable although some progress has been made with asymptotic formulas.

Harborth and I investigated [16] extremal animals with respect to various parameters. For example among the five animals (Figure 3) with four cells, it is obvious that all of them except Fatty have 10 nodes when regarded as graphs, and have perimeter 10, while for Fatty these numbers are 9 nodes and perimeter 8. This illustrates mathematical research suggested by biology.

Martin Gardner [4] and I [14] summarized some of the games which I discovered concerning animals. These games may be regarded as generalizations of «Naughts and Crosses».

B2. Ecology.

In an *ecological system*, we have a digraph in which the nodes are various species of animals, possibly including vegetation, and an arc from u to v indicates that species u eats species v. Many years ago, when my children were small and I read books to them, I found in the Ann Arbor Public Library a book with such a digraph (actually, an oriented graph as there can be no symmetric pair of arcs) drawn on the front cover. This booklet was the stimulus for my note [9], «Who eats whom?», which the mathematical biologist Joel Cohen certified was the first of many papers to propose digraphs as a mathematical model for ecology.

At that time I had recently contributed formulations of status and its directional dual, contrastatus [8], in a digraph regarded as an organization chart (of a company or a university department or a governmental agency). The *status* $s(u)$ of a node u in a digraph D may be defined as the sum of the distances $d(u,v)$ *from* u to all other nodes v. This study was suggested by the popular book, «Parkinson's Law», [19].

On applying these concepts to an undirected connected graph G, the set of all nodes of minimum status has been called the *median* of a graph. This is one of several kinds of graph centrality presented in our very recent book [2] on distance in graphs.

4. Graph Models in Chemistry.

My first paper on this application area [1] was written with the Romanian chemist A.T. Balaban; it appeared in the book he edited on the subject. More recently my chemistry-partner is Paul Mezey with whom an entire book on «Graph Theory and Chemistry» is planned, in addition to our two papers [17, 18] to date.

There exists a book [3] on organic chemistry with 16 chapters, each of which is titled with the diagram of a polyhex, the first four of which are shown in Figure 4.

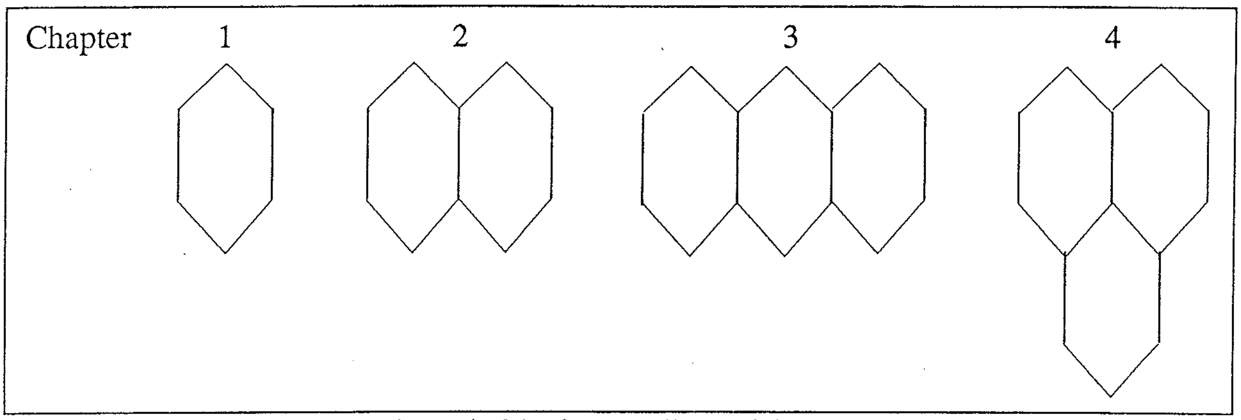

Figure 4 - The four smallest polyhexes.

Clearly this section can be expanded to an entire book. (indeed this applies to each of the two preceding sections as well). In fact, virtually every topic in the book [11] suggests a realization in chemistry. For example two different graphs with the same partition of $2q$ (double the number of edges) as the sum of the degrees of the nodes can represent a graph-reaction abstraction of a simple chemical reaction.

5. Other application areas.

Networks and graphs occur naturally in all fields which exhibit some structure. Instead of the above choice of A, B, C subjects, one might have chosen Architecture, Botany and Computer Science. The examples would have been different but the same theme would be apparent.

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