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The description and group properties of linear graphs

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Abstract. A new method for the identification and ordering of linear graphs is described. The method pays particular attention to the group properties of graphs and is easy to adapt for use with electronic computers.

1. Introduction

In this paper a method is described for the ordering and identification of linear graphs. As an integral part of the method, representations of the point group and bond group of any graph are produced. Although the nomenclature of linear graphs is a general problem in graph theory, we have approached this study from the fact that graphs occur in the investigation of many-body systems by the method of exact series expansion (Uhlenbeck and Ford 1962, Sykes *et al* 1966, Domb and Green 1974, Sykes *et al* 1974). The problem of graph identification arises in the method of exact series expansion in the following way. Each graph represents a contribution to a series expansion of some quantity of physical interest. Each contribution is a set of numbers which are associated with the graph. Some of these numbers vary from problem to problem whereas others are invariant. It is convenient to calculate the invariant quantities separately and store them for use with a variety of problems; that is, one creates a graph library. It is obvious that to retrieve the numbers from the library, one requires an unambiguous description of each entry. Some of these graph libraries are quite large, containing several tens of thousands of entries. Any practicable method of handling such data must rely on electronic computers.

There are several methods in existence which treat the problem of identification of graphs. The method with the widest appeal is to draw a diagram of each graph (eg Harary 1969, Uhlenbeck and Ford 1962). Though vivid, this method is cumbersome and unsuited to electronic computers.

For many physical applications, particularly problems for which it is natural to classify graphs by their number of edges, it is advantageous to consider the identification problem in two parts First, one identifies the graph *topology* and second the *realization* of the topology. If one defines the *valence* of a vertex of a linear graph as the number of bonds incident at the vertex, one may define topology and realization as follows. A topology is a collection of vertices and *bridges* (bonds) with the property that no vertex is of valence 2. In topologies, loops and multiple bridges are allowed. A realization is obtained from the topology by inserting vertices of valence 2 in the bridges of the topology. A realization is a linear graph. Non-isomorphic realizations of the same topology are said to be homeomorphs. The concept of topology is useful in situations where graphs are grouped by the number of edges they contain and where one is interested in properties which depend only on the basic topology of the graph.

An early identification method assigned an arbitrary name to each topology and associated with each topology a set of rules whereby the realizations could be identified (Sykes *et al* 1966, Essam and Sykes 1966). It is very difficult to use this method with computers but the names of the topologies are still used in manual or informal work. Nagel (1966) has proposed a system of nomenclature for graph topologies which has been extensively used on electronic computers by Heap (1967, 1969). The scheme to be described bears several points of similarity to that of Nagel and Heap. However, the method we have constructed is more direct and adaptable to a variety of situations. Furthermore, identification of the realizations is easily included and the symmetry properties of topologies and realizations are investigated in detail.

We shall first give a formal description of the method, postponing examples to appendix 1. A few interesting points about the application to electronic computers are given in appendix 2.

2. Method

The problem of defining a unique description of a linear graph is solved by giving a unique or *canonical* description to the graph topology by a method which constructs a representation of the bridge group of the topology. Any realization can then be uniquely described by using the bridge group of the topology. The realization is represented by the set of bridge lengths, where the length of a bridge is the number of edges it contains. We describe first the canonical description of a topology.

The v vertices and the b bridges of the topology are arbitrarily labelled by the integers $\{1, 2, \ldots, v\}$ and $\{1, 2, \ldots, b\}$ respectively. This description will be called the *initial description* and it can be represented by the set of b number pairs

$$((x_{11}, x_{12}), (x_{21}, x_{22}), \ldots, (x_{b1}, x_{b2})).$$

The elements x_{i1} and x_{i2} of the ith pair represent the vertex labels of the vertices joined by the bridge labelled i. The elements of each pair are ordered so that $x_{i1} \leqslant x_{i2}$. A permutation of b ordered pairs of integers with this form will be called a $b2$ *tuple*. (Each $b2$ tuple is a linear representation of the incidence matrix of the topology.) A *vertex tuple* X is a permutation of the first v positive integers. Associated with the initial description are the vertex tuple $(1, 2, \ldots, v)$ and the bridge tuple $(1, 2, \ldots, b)$.

It is convenient at this stage to define an ordering relation between sets. If

$$C = \{c_1, c_2, \ldots, c_n\} \qquad \text{and} \qquad D = \{d_1, d_2, \ldots, d_n\}$$

where c_i and d_i $(1 \leqslant i \leqslant n)$ are integers, then $C \prec D$ (C precedes D) (i) if $c_1 < d_1$, or (ii) if $c_i < d_i$ when $i \in \{2, 3, \ldots, n-1\}$ and $c_j = d_j$ for all $j \in \{1, 2, \ldots, i-1\}$, or (iii) if $c_n \leqslant d_n$ when $c_j = d_j$ for all $j \in \{1, 2, \ldots, n-1\}$. This definition is readily extended to $b2$ tuples as follows. If

$$C = ((c_{11}, c_{12}), (c_{21}, c_{22}), \ldots, (c_{n1}, c_{n2}))$$

and

$$D = ((d_{11}, d_{12}), (d_{21}, d_{22}), \ldots, (d_{n1}, d_{n2}))$$

where c_{ij} and d_{ij} $(1 \leqslant i \leqslant n,\ 1 \leqslant j \leqslant 2)$ are integers, then $C \prec D$ (i) if $c_{11} < d_{11}$ (or if

$c_{11} = d_{11}, c_{12} < d_{12}$), or (ii) if $c_{i1} < d_{i1}$ (or if $c_{i1} = d_{i1}, c_{i2} < d_{i2}$) when $i \in \{2, 3, \ldots, n-1\}$ and $c_{j1} = d_{j1}$, $c_{j2} = d_{j2}$ for all $j \in \{1, 2, \ldots, i-1\}$, or (iii) if $c_{n1} < d_{n1}$ (or if $c_{n1} = d_{n1}$, $c_{n2} \leqslant d_{n2}$) when $c_{j1} = d_{j1}$ and $c_{j2} = d_{j2}$ for all $j \in \{1, 2, \ldots, n-1\}$. In both cases, if $C \prec D$ and $D \prec C$ then C and D are *identical*, written $C = D$.

The initial description of the topology is arbitrary. Corresponding to each bridge tuple is a permutation of the b number pairs of the initial description. We obtain therefore a class of $b2$ tuples containing $b!$ members. The members of this class are ordered so that $B_1 \prec B_2 \prec B_3 \ldots \prec B_{b!}$. It will be found that the ordering divides the class of $b2$ tuples into subclasses $\mathscr{B}_k$ all of whose members are identical. Each subclass contains the same number S_2 of elements which is the order of the *multibridge* group of the topology. The bridge tuples associated with the $b2$ tuples are also grouped in classes $\mathscr{Y}_k$ to correspond with the $\mathscr{B}_k$. Each $\mathscr{Y}_k$ is a representation of the multibridge group of the topology. This group accounts for the symmetry elements due to multiple bridges between two vertices. The subclasses $\mathscr{B}_k$ are ordered so that if $C \in \mathscr{B}_k$ and $D \in \mathscr{B}_l$ and $C \prec D$ then $k \leqslant l$. If $B \in \mathscr{B}_1$ then B is known as a *minimum description.*

The minimum description obtained above was found from the initial vertex labelling corresponding to the vertex tuple $(1, 2, \ldots, v)$. There are $v!$ ways of labelling the vertices of the topology. Each labelling is described by a vertex tuple X_i $(1 \leqslant i \leqslant v!)$. Corresponding to each X_i we may find a minimum description B_i and an associated representation $\mathscr{Y}_i$ of the multibridge group. It will be found that the class of minimum descriptions can be divided into subclasses $\mathscr{C}_k$ whose members are identical. The $\mathscr{C}_k$ are ordered so that if $C \in \mathscr{C}_k$ and $D \in \mathscr{C}_l$ and $k < l$ then $C \prec D$. Each subclass $\mathscr{C}_k$ contains the same number of elements S_1 which is the order of the *vertex group* of the topology. Associated with each $\mathscr{C}_k$ is a class of vertex tuples $\mathscr{X}_k = \{X_{k,1}, \ldots, X_{k,S_1}\}$ and a class of bridge tuples $\mathscr{Z}_{k,i}$ is associated with each $X_{k,i}$. If $B \in \mathscr{C}_1$ then B is the *canonical description* of the topology. The class of vertex tuples $\mathscr{H} = \mathscr{X}_1$ is a representation of the vertex group of the topology and the class of bridge tuples $\mathscr{G} = \cup_{i=1}^{S_1} \mathscr{Z}_{1i}$ is a representation of the bridge group of the topology. The latter group is of order $S_1 S_2$.

As defined above, the classes $\mathscr{H}$ and $\mathscr{G}$ contain information concerning the initial labelling of the topology. They are known as the *un-normalized symmetry rules.* We obtain the *normalized* symmetry rules $\mathscr{H}^*$ and $\mathscr{G}^*$ by choosing to represent one member of $\mathscr{H}$ by $(1, 2, \ldots, v)$ and one member of $\mathscr{G}$ by $(1, 2, \ldots, b)$ and renumbering the remaining members accordingly. This procedure chooses the identity element for each group. The information about the initial description is lost. The binary operation $\otimes$ for the group $\mathscr{H}^*$ is easily defined. If $X_1, X_2 \in \mathscr{H}^*$ and

$$X_1 = \{x_1^{(1)}, x_2^{(1)}, \ldots, x_v^{(1)}\}, \qquad X_2 = \{x_1^{(2)}, x_2^{(2)}, \ldots, x_v^{(2)}\},$$

then

$$X_1 \otimes X_2 = \{x^{(2)}_{x_1^{(1)}}, x^{(2)}_{x_2^{(1)}}, \ldots, x^{(2)}_{x_v^{(1)}}\}.$$

A similar definition holds concerning $\mathscr{G}^*$. We define the group $\mathscr{H}^*$ here for completeness although it is not used in the subsequent discussion.

We now use the bridge group $\mathscr{G}^*$ to define the canonical description of a realization of the topology. A realization of the topology is formed by associating an integer weight r_j $(1 \leqslant j \leqslant b)$ with each bridge of the topology. The realizations represent linear graphs and the weights represent the number of edges of the graph which constitute each bridge of the topology. Each realization may be uniquely described by operating with the bridge group $\mathscr{G}^*$ on the realization description $R = (r_1, r_2, \ldots, r_b)$. Thus if

$Y_i \in \mathscr{G}^*$, for $1 \leqslant i \leqslant S_1 S_2$, then the tuples $R_i = Y_i \otimes R$ are all descriptions of the realization. The R_i are ordered so that if $j < k$ then $R_j \prec R_k$. The set R_1 is then the *canonical description* of the realization. A representation of the symmetry group of the realization is given by the class of bridge tuples $Y_j\,(1 \leqslant j \leqslant \sigma)$ such that $Y_j \otimes R = R_1$. The order σ of this group is the symmetry number of the realization.

The relation $\prec$ can be used to order topologies and to order the realizations of a topology. The customary order for topologies is based on the scheme of Nagel and Heap and is still extensively used. However the realizations of a topology are arranged first by the total number of edges and second by the relation $\prec$. The ordering of the realizations greatly facilitates list searching.

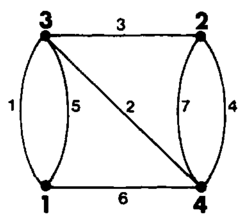
3. Summary and comments

We have defined the canonical description of a toplogy as the minimum of all possible *b*2 tuples. The method of finding the canonical description also produces representations of the vertex and bridge groups of the topology. The bridge group is used to find the canonical description of a realization of the topology.

The method can be applied *directly* to linear graphs. The vertices of the graph are labelled and the initial *b*2 tuple is written down. The minimum *b*2 tuple is then found in the manner described above. Each *b*2 tuple is a representation of the incidence matrix of the graph. This gives a different classification of graphs from that already described. The extension of this method to digraphs is trivial. The direct method also obviates the need to make the polygons a special case. By convention the polygons have the toplogy described by the *b*2 tuple ((1, 1)).

Appendix 1. Example

Suppose we wish to canonize the topology



The initial labelling is shown. The initial vertex tuple, bridge tuple and *b*2 tuple are (1, 2, 3, 4), (1, 2, 3, 4, 5, 6, 7) and ((1, 3), (3, 4), (2, 3), (2, 4), (1, 3), (1, 4), (2, 4)) respectively. The minimum description with this vertex tuple is ((1, 3), (1, 3), (1, 4), (2, 3), (2, 4), (2, 4), (3, 4)) and the corresponding representation of the multibridge group is given by the four bridge tuples

(1, 5, 6, 3, 4, 7, 2)

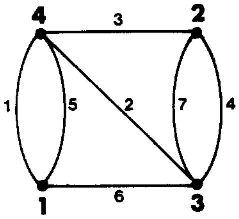
(1, 5, 6, 3, 7, 4, 2)

(5, 1, 6, 3, 4, 7, 2)

(5, 1, 6, 3, 7, 4, 2)

The multibridge group takes account of the symmetry due to the multiple bridges between vertices 1 and 3 and between vertices 2 and 4. The order of the group is $4 = 2!2!$

The vertex tuple is now changed to $(1, 2, 4, 3)$ to produce the following labelled topology:



The minimum description is now

$$((1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4), (3, 4))$$

and the multibridge group is represented by

$$(6, 1, 5, 4, 7, 3, 2)$$
$$(6, 1, 5, 7, 4, 3, 2)$$
$$(6, 5, 1, 4, 7, 3, 2)$$
$$(6, 5, 1, 7, 4, 3, 2).$$

We run through the 24 vertex tuples X_1 to X_{24} to produce the 24 minimum descriptions C_1 to C_{24} shown in table 1. By inspection the minimum descriptions are identical in pairs, eg $C_1 = C_8$, $C_2 = C_7$. By ordering the minimum descriptions we see that the canonical description of the topology is given by C_{11} or C_{22}; that is,

$$((1, 2), (1, 2), (1, 3), (1, 4), (2, 3), (3, 4), (3, 4)).$$

The vertex group $\mathscr{H}$ is represented by the class $\mathscr{X}_1 = \{X_{11}, X_{22}\}$, that is

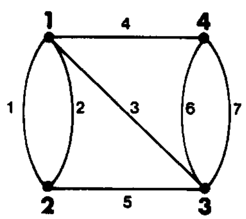
$$\{(2, 4, 1, 3), (4, 2, 3, 1)\}.$$

Associated with X_{11} and X_{22} are the multibridge groups represented by the following classes:

$$\mathscr{X}_{1,1} = \{(1, 5, 2, 3, 6, 4, 7) \quad (1, 5, 2, 3, 6, 7, 4) \quad (5, 1, 2, 3, 6, 4, 7) \quad (5, 1, 2, 3, 6, 7, 4)\}$$

$$\mathscr{X}_{1,2} = \{(4, 7, 2, 6, 3, 1, 5) \quad (4, 7, 2, 6, 3, 5, 1) \quad (7, 4, 2, 6, 3, 1, 5) \quad (7, 4, 2, 6, 3, 5, 1)\}.$$

The group $\mathscr{G}$ is represented by $\mathscr{X}_{1,1} \cup \mathscr{X}_{1,2}$. The normalized group $\mathscr{H}^*$ is represented by the class $\{(1, 2, 3, 4), (2, 1, 4, 3)\}$, the members of which correspond to the vertex labellings



and

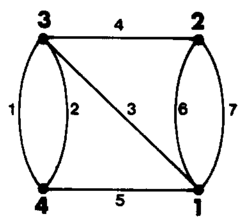
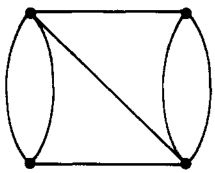


Table 1. The 24 vertex tuples and minimum descriptions of the topology



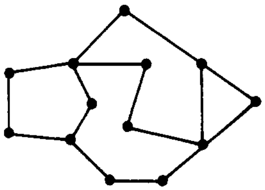
	Vertex tuple		Minimum description
X_1	(1, 2, 3, 4)	C_1	((1, 3), (1, 3), (1, 4), (2, 3), (2, 4), (2, 4), (3, 4))
X_2	(1, 2, 4, 3)	C_2	((1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4), (3, 4))
X_3	(1, 3, 2, 4)	C_3	((1, 2), (1, 2), (1, 4), (2, 3), (2, 4), (3, 4), (3, 4))
X_4	(1, 3, 4, 2)	C_4	((1, 2), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4), (3, 4))
X_5	(1, 4, 2, 3)	C_5	((1, 2), (1, 2), (1, 3), (2, 3), (2, 4), (3, 4), (3, 4))
X_6	(1, 4, 3, 2)	C_6	((1, 2), (1, 3), (1, 3), (2, 3), (2, 4), (2, 4), (3, 4))
X_7	(2, 1, 3, 4)	C_7	((1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4), (3, 4))
X_8	(2, 1, 4, 3)	C_8	((1, 3), (1, 3), (1, 4), (2, 3), (2, 4), (2, 4), (3, 4))
X_9	(2, 3, 1, 4)	C_9	((1, 2), (1, 2), (1, 3), (1, 4), (2, 4), (3, 4), (3, 4))
X_{10}	(2, 3, 4, 1)	C_{10}	((1, 2), (1, 3), (1, 3), (1, 4), (2, 4), (2, 4), (3, 4))
X_{11}	(2, 4, 1, 3)	C_{11}	((1, 2), (1, 2), (1, 3), (1, 4), (2, 3), (3, 4), (3, 4))
X_{12}	(2, 4, 3, 1)	C_{12}	((1, 2), (1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (3, 4))
X_{13}	(3, 1, 2, 4)	C_{13}	((1, 2), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4), (3, 4))
X_{14}	(3, 1, 4, 2)	C_{14}	((1, 2), (1, 2), (1, 4), (2, 3), (2, 4), (3, 4), (3, 4))
X_{15}	(3, 2, 1, 4)	C_{15}	((1, 2), (1, 3), (1, 3), (1, 4), (2, 4), (2, 4), (3, 4))
X_{16}	(3, 2, 4, 1)	C_{16}	((1, 2), (1, 2), (1, 3), (1, 4), (2, 4), (3, 4), (3, 4))
X_{17}	(3, 4, 1, 2)	C_{17}	((1, 2), (1, 3), (1, 3), (1, 4), (2, 3), (2, 4), (2, 4))
X_{18}	(3, 4, 2, 1)	C_{18}	((1, 2), (1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4))
X_{19}	(4, 1, 2, 3)	C_{19}	((1, 2), (1, 3), (1, 3), (2, 3), (2, 4), (2, 4), (3, 4))
X_{20}	(4, 1, 3, 2)	C_{20}	((1, 2), (1, 2)' (1, 3), (2, 3), (2, 4), (3, 4), (3, 4))
X_{21}	(4, 2, 1, 3)	C_{21}	((1, 2), (1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (3, 4))
X_{22}	(4, 2, 3, 1)	C_{22}	((1, 2), (1, 2), (1, 3), (1, 4), (2, 3), (3, 4), (3, 4))
X_{23}	(4, 3, 1, 2)	C_{23}	((1, 2), (1, 3), (1, 4), (1, 4), (2, 3), (2, 3), (2, 4))
X_{24}	(4, 3, 2, 1)	C_{24}	((1, 2), (1, 3), (1, 3), (1, 4), (2, 3), (2, 4), (2, 4))

respectively. The normalized group $\mathscr{G}^*$ is represented by

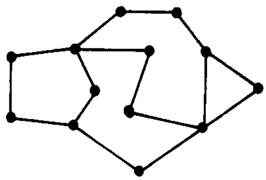
$$\{(1, 2, 3, 4, 5, 6, 7),$$
$$(1, 2, 3, 4, 5, 7, 6),$$
$$(2, 1, 3, 4, 5, 6, 7),$$
$$(2, 1, 3, 4, 5, 7, 6),$$
$$(6, 7, 3, 5, 4, 1, 2),$$
$$(6, 7, 3, 5, 4, 2, 1),$$
$$(7, 6, 3, 5, 4, 1, 2),$$
$$(7, 6, 3, 5, 4, 2, 1)\}$$

corresponding to the bridge labelling shown above.

To illustrate the canonical description of a realization, suppose we are given the following realizations of the topology;



(1)



(2)

Each realization has three bridges of length 3, three bridges of length 2 and one bridge of length 1. Corresponding to the canonical description of the topology we describe the realizations by

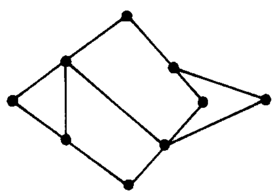
$$R^{(1)} = (3, 2, 3, 2, 3, 1, 2) \qquad \text{and} \qquad R^{(2)} = (3, 2, 3, 3, 2, 1, 2).$$

By operating on $R^{(1)}$ and $R^{(2)}$ with the group $\mathscr{G}^*$ we obtain eight equivalent descriptions of each realization, namely

$$R_1^{(1)} = (3, 2, 3, 2, 3, 1, 2) \qquad \text{and} \qquad R_1^{(2)} = (3, 2, 3, 3, 2, 1, 2)$$
$$R_2^{(1)} = (3, 2, 3, 2, 3, 2, 1) \qquad\qquad R_2^{(2)} = (3, 2, 3, 3, 2, 2, 1)$$
$$R_3^{(1)} = (2, 3, 3, 2, 3, 1, 2) \qquad\qquad R_3^{(2)} = (2, 3, 3, 3, 2, 1, 2)$$
$$R_4^{(1)} = (2, 3, 3, 2, 3, 2, 1) \qquad\qquad R_4^{(2)} = (2, 3, 3, 3, 2, 2, 1)$$
$$R_5^{(1)} = (1, 2, 3, 3, 2, 3, 2) \qquad\qquad R_5^{(2)} = (1, 2, 3, 2, 3, 3, 2)$$
$$R_6^{(1)} = (1, 2, 3, 3, 2, 2, 3) \qquad\qquad R_6^{(2)} = (1, 2, 3, 2, 3, 2, 3)$$
$$R_7^{(1)} = (2, 1, 3, 3, 2, 3, 2) \qquad\qquad R_7^{(2)} = (2, 1, 3, 2, 3, 3, 2)$$
$$R_8^{(1)} = (2, 1, 3, 3, 2, 2, 3) \qquad\qquad R_8^{(2)} = (2, 1, 3, 2, 3, 2, 3).$$

The canonical description of (1) is $R_6^{(1)}$ and the canonical description of (2) is $R_6^{(2)}$. The symmetry number of both these realizations is 1.

To illustrate the effects of symmetry with respect to realizations, let us consider the realization



(3)

The eight equivalent descriptions are

$$R_1^{(3)} = (2, 1, 1, 2, 2, 2, 2)$$
$$R_2^{(3)} = (2, 1, 1, 2, 2, 2, 2)$$
$$R_3^{(3)} = (1, 2, 1, 2, 2, 2, 2)$$

$R_4^{(3)} = (1, 2, 1, 2, 2, 2, 2)$

$R_5^{(3)} = (2, 2, 1, 2, 2, 2, 1)$

$R_6^{(3)} = (2, 2, 1, 2, 2, 1, 2)$

$R_7^{(3)} = (2, 2, 1, 2, 2, 2, 1)$

$R_8^{(3)} = (2, 2, 1, 2, 2, 1, 2).$

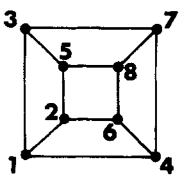
The canonical description is given by $R_3^{(3)}$ or $R_4^{(3)}$. The symmetry group of the realization is represented by the third and fourth members of $\mathscr{G}^*$ and the symmetry number is 2.

Appendix 2. Some practical points

The canonization procedure has been translated into a FORTRAN computer program. The program finds the canonical description of any topology and the un-normalized bridge and vertex symmetry rules. It calculates the normalized symmetry rules on request. This option allows a saving in storage space, though the program is not particularly large. It requires approximately 12 K bytes (about 5000 words) on an IBM 360 machine. The program can be used as a subroutine in more complex programs. Readers interested in using the program are asked to contact the author.

To increase the speed of the program a number of subterfuges have been used. First, the innermost cycle of the program is that which finds the minimum description for each vertex tuple. If the $b2$ tuples are considered merely as numbers of order λ^{2b} where λ is some base ($\lambda > v$), then the minimum $b2$ tuple is the smallest of such numbers. The program is written to find the minimum by rearranging the elements of the $b2$ tuple. Thus the need to run through all $b!$ bridge tuples is obviated. However, the multibridge symmetry is not included. This is easy to identify and include in the final stage of the program.

It is also very inefficient for the program to scan all $v!$ vertex tuples. The innermost loop is quite substantial and the fewer times it is entered the better. It is possible to make very large savings in computer time with a little care. It has been noticed that the canonical description of a connected topology has the property that vertex 2 is connected to vertex 1, vertex 3 to either 2 or 1, vertex 4 to either 3, 2 or 1 and so on. The proof of this statement is straightforward though too lengthy to include here. Thus having chosen vertex 1, vertex 2 must be connected to 1 and the choice of vertex 2 made accordingly. If one chooses vertex 1 intelligently, and there are a number of guidelines for one's choice, the canonical description can be found with ease. For example, the program finds the canonical description and the symmetry rules for the cube



which has symmetry number 48, on entering the innermost cycle 96 times. This compares with $8! = 40\,320$ possible vertex tuples. An additional logical path has been included in the program to take care of disconnected topologies.

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