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ON GRAPHS AND THEIR ENUMERATION

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Already in the nineteenth century it was recognized that chemical molecules can be described in a sense by graphs, the points of which represent the atoms, and the lines of which represent the bonds. And very soon the question was raised, how many such graphs exist which are essentially different but which illustrate in this way molecules with the same brutto formula. This was before mathematicians really started developing graph theory so that in fact one may say that considerations of chemists initiated the theory of graphs and the theory of their enumeration.

The problem of enumerating and constructing all the different graphs which represent molecules with a given brutto fomula is still far from a satisfactory solution but along mentioning the basic concepts of the theory of graphs and their enumeration I would like to show how at least it can be attacked.

In order to do this we need at first state this problem in terms of a mathematical concept which is flexible enough so that it covers the various graph theoretical concepts which are used in such applications of graph theory as there are the usual graphs with undirected lines, without loops and without multiple lines or as in other cases the multigraphs which have undirected lines and no loops, too, but where multiple lines are allowed, as well as it should cover the concept of directed graphs and graphs with loops.

It will turn out that the concept of enumeration of symmetry types of functions between two finite sets yields what we need in each case if the two sets are suitably chosen.

1. Functions between finite sets

We assume that we are given two finite nonempty sets, say X and Y. We denote by Y^X the set of all the mappings f from X to Y, for short:

$$Y^X = \{f \mid f:X\to Y\}.$$

Example: Let $P=\{p,q,r,s\}$ denote the set of points of a labeled graph, say of

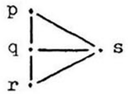


Fig. 1

We take for X the set $P^{\{2\}}$ of the 6 pairs of points, i.e.

$$X = \{\{p,q\},\{p,r\},\{p,s\},\{q,r\},\{q,s\},\{r,s\}\}.$$

For Y we take

$$Y = \{0,1\}.$$

Then a mapping $f:X \to Y$ may be considered as the labeled graph which has P as point set and where $f(x)=0$ if and only if the pair x of points is not connected and where $f(x)=1$ if and only if the pair x is connected. Then e.g. the function

$$f: \begin{array}{lll} \{p,q\} \mapsto 1 & \{q,r\} \mapsto 1 & \\ \{p,r\} \mapsto 0 & & \{r,s\} \mapsto 1 \\ \{p,s\} \mapsto 1 & \{q,s\} \mapsto 1 & \end{array}$$

yields the graph of fig. 1.

But this concept covers not only graphs with no multiple lines. Just by extending Y, multiple lines may come in.

Example: We take P and $X=P^{\{2\}}$ as above, but now we put $Y=\{0,1,2\}$ and see that

$$f: \begin{array}{lll} \{p,q\} \mapsto 2 & \{q,r\} \mapsto 2 & \\ \{p,r\} \mapsto 0 & & \{r,s\} \mapsto 1 \\ \{p,s\} \mapsto 1 & \{q,s\} \mapsto 1 & \end{array}$$

yields the multigraph of the Königsberg bridge problem:

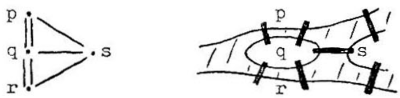
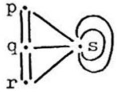


Fig. 2

It is clear that by taking $X=P^{\{2\}}$ and $Y=\{0,1,\ldots,k\}$ we obtain multigraphs with up to k-fold lines. Still loops do not occur. But once we take for X the union of $P^{\{2\}}$ and P, i.e. if we put $X=P^{\{2\}} \cup P$ and $Y=\{0,1,\ldots,k\}$, the k-fold lines as well as k-fold loops may occur like in

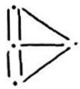


of $\{0,1,2\}^{P^{\{2\}}} \cup P$

Fig. 3

2. Symmetry types of functions

We are mostly interested in unlabeled graphs so that we are not willing to distinguish the following two graphs



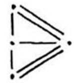
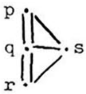
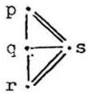


Fig. 4

which arise from the functions

f_1: 

and f_2: 

by just delabeling.

We first notice that we obtain f_2 from f_1 by permuting the points q and s or by exchanging the pairs of points

$\{p,q\}$ and $\{p,s\}$

$\{q,r\}$ and $\{r,s\}$.

In other words, f_2 is the same as first applying a certain permutation π onto $P^{\{2\}}$ and then applying f_1, i.e. $f_2=f_1\circ\pi$.

This leads to the following definition: Once we are given a permutation group H on X, the two elements f_1, f_2 in Y^X are called <u>equivalent with respect to</u> H (for short: $f_1 \sim_H f_2$) if and only if there exists a π in H which satisfies

$$f_2 = f_1\circ\pi.$$

<u>Example:</u> We take again $P=\{p,q,r,s\}$ and $X=P^{\{2\}}$ and $Y=\{0,1,2\}$. And we ask, how H has to be defined in order that f_2 and f_1 are equivalent if and only if they represent the same graph.

Two labeled graphs with the same set P of points represent the same graph if and only if one of them can be obtained from the other by a permutation σ of P.

The permutations σ of P form the symmetric group S_P of P and they induce permutations π of the set $P^{\{2\}}$ of the pair~ of points. E.g.

σ of S_P induces π as follows: If x, y are elements of P, then we define π by

$$\pi\{x,y\} = \{\sigma(x), \sigma(y)\} .$$

The group of all the π's is denoted by $S_P^{\{2\}}$ and called the <u>pair group corresponding to</u> S_P.

Hence f_1 and f_2 of $Y^{P^{\{2\}}}$ represent the same graph if and only if they are equivalent with respect to the pair group $S_P^{\{2\}}$.

Let us return to the general case, where Y^X is considered together with a permutation group H on X and the equivalence as defined above. The equivalence relation dissects Y^X completely into pairwise disjoint subsets, the equivalence classes or better say <u>the symmetry types of functions</u> from X to Y with respect to H.

Using this notation we are now in a position to give a precise definition of graphs:

<u>Definition</u>: The <u>graphs</u> with point set P, without loops and with up to k-fold lines are the symmetry types of functions f from $X=P^{\{2\}}$ to $Y=\{0,1,\dots,k\}$ and with respect to the pair group $H = S_P^{\{2\}}$.

How graphs with loops can be defined in this way is now obvious, also how <u>directed graphs</u> can be defined (instead of the set $P^{\{2\}}$ of unordered pairs choose the set P^2 of ordered pairs of points).

3. Enumeration of symmetry types

The definition of graphs with point set P at the end of the preceding section has shown that it is of interest to attack the following three enumeration problems concerning the symmetry types of functions f in Y^X with respect to a permutation group H on X:

(i) Evaluate the number of symmetry types.

(ii) Evaluate the number of symmetry types of prescribed kind $(k_1,\dots,k_{|Y|})$, where k_i denotes the number of values which are equal to $y_i \in Y$.

(iii) Construct for each type of prescribed kind $(k_1,\dots,k_{|Y|})$ a function of that type.

These problems are of increasing difficulty.

The first problem is solved by <u>Burnside's lemma</u>, which gives us the number of orbits of a permutation group. It says that the number of symmetry types is equal to

$$\frac{1}{|H|}\sum_{\pi\in H} b_1(\pi),$$

where $b_1(\pi)$ is the number of functions $f\in Y^X$ which satisfy

$$f = f\circ\pi.$$

If $\pi\in H$ is a product of $c(\pi)$ cyclic factors, like e.g.

$$\pi = \begin{pmatrix}1&2&3&4&5&6&7&8\\5&3&2&1&4&7&8&6\end{pmatrix} = (154)(23)(678)$$

is a product of 3 cyclic factors so that $c(\pi)=3$, then it is easy to see that

$$b_1(\pi) = |Y|^{c(\pi)}.$$

Hence the number of symmetry types of Y^X with respect to H amounts to

$$\frac{1}{|H|}\sum_{\pi\in H} |Y|^{c(\pi)}.$$

This is the well known solution of problem (i).

Problem (ii) is solved with the aid of the <u>cycle-index</u> polynomial which corresponds to H:

$$Z(H) = \frac{1}{|H|}\sum_{\pi\in H} x_1^{a_1(\pi)} \cdots x_{|X|}^{a_{|X|}(\pi)},$$

where $a_i(\pi)$ denotes the number of cyclic factors of π which are of length i, for $1\le i\le |X|$.

If in this polynomial Z(H) we substitute the polynomial

$$y_1^i + \dots + y_{|Y|}^i$$

for x_i, we obtain the polynomial

$$Z(H\,|\,y_1+\dots+y_{|Y|}) = \frac{1}{|H|}\sum_{\pi\in H} (y_1^1+\dots+y_{|Y|}^1)^{a_1(\pi)} \cdots (y_1^{|X|}+\dots+y_{|Y|}^{|X|})^{a_{|X|}(\pi)}$$

and the famous <u>theorem of Pólya</u> says that the number of symmetry types of functions of kind $(k_1,\dots,k_{|Y|})$ is just the coefficient of

$$y_1^{k_1}\cdots y_{|Y|}^{k_{|Y|}}$$

in $Z(H\,|\,y_1+\dots+y_{|Y|})$.

Hence problem (ii) is solved once we know the cycle-index of H.

Problem (iii) is the most difficult one as well as the most interesting one.

It can be shown that one can obtain a complete system of representatives of symmetry types of kind $(k_1,\dots,k_{|Y|})$ from a complete system of representatives of so-called double-cosets

$$S_{k_1} \times \dots \times S_{k_{|Y|}} \gamma H$$

of $S_{k_1} \times \dots \times S_{k_{|Y|}}$ and H in S_X. $S_{k_1} \times \dots \times S_{k_{|Y|}}$ is a direct product of symmetric groups S_{k_i}, and the double-cosets are the following subsets of the symmetric group S_X on X:

$$S_{k_1} \times \dots \times S_{k_{|Y|}} \gamma H = \{\delta \mid \delta = \alpha\gamma\beta, \ \alpha \in S_{k_1} \times \dots \times S_{k_{|Y|}}, \beta \in H\}.$$

There are in fact algorithms available which yield such systems of representatives of double-cosets. They are quite complicated to implement and need big computers.

Using such a program one may start with first constructing a complete system of graphs with prescribed multiplicities of bonds and then extract from these the ones which are of interest for the applications in question.

This is of course a huge waste of computer time but it shows how the problem can be embedded in the mathematical concept of enumeration of symmetry types of functions. If one is interested in a special problem like enumeration or even construction of a certain kind of isomeres say, one of course should try to attack the problem directly so that no graphs will be constructed which have to bee thrown out later on. Still one step will be a construction of symmetry types, as can be seen from the papers published by the people from the Stanford group which are given below.

Brown, H./Hjelmeland, L./Masinter, L.: Constructive graph labeling using double cosets. Discrete Math. 7 (1974), 1-30.

Brown, H./Masinter, L.: An Algorithm for the construction of the graphs of organic molecules. Discrete Math. 8 (1974), 227-244