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ON GRAPHS AND THEIR ENUMERATION II

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During the microsymposium on graph theory in chemistry which gave rise to the publication of MATCH it turned out that graphs and their enumeration are a useful concept in chemistry, so that it seems worthwhile to continue the introductory remarks on this theory which I made in MATCH 1.

Being a mathematician, my main task seems to me to be that I should point to mathematical concepts which can be used successfully in this context. The methods which can be recommended should on the one hand be general enough so that they cover the problems arising in applications (as far as I know them) and on the other hand they should not be too general, so that the necessary mathematical tools are familiar enough to the people who might like to apply them.

Thus let me point out, how Pólya's enumeration theory can be comprised in representation theory of finite groups and in particular of symmetric groups so that character tables and all that turn out to be useful tools here as well. I should not forget to mention that this embedding of enumeration theory into representation theory raises some hitherto unsolved problems in representation theory.

Before we start, let us recall from part I that we are dealing with given finite sets X and Y and that we consider the set

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

which consists of all the mappings f from X to Y. Furthermore, we are given a permutation group H acting on X. This group induces an equivalence relation "$\sim$" on Y^X : $f_1 \in Y^X$ is called equivalent to $f_2 \in Y^X$ (for short: $f_1 \sim f_2$) if and only if there exists a $\pi \in H$ such that

$$f_1 = f_2 \circ \pi^{-1},$$

(where $f_2 \circ \pi^{-1}$ means composition of f_2 and π^{-1}, i.e. for each $x \in X : (f_2 \circ \pi^{-1})(x) = f_2(\pi^{-1}(x))$).

Our most prominent example was: If P denotes a set of points, then we take $X = P^{\{2\}}$, the set of pairs of points, put $Y = \{0,1\}$, and take $H = S_P^{\{2\}}$, the group induced by the symmetric group S_P on the set $P^{\{2\}}$. In this case the equivalence classes can be interpreted as the isomorphism types of graphs without loops and single edges only.

1. Formulation in terms of group theory

For a fixed $\pi \in H$, the mapping

$$\hat{\pi} : f \longmapsto f \circ \pi^{-1},$$

which maps $f \in Y^X$ onto $f \circ \pi^{-1} \in Y^X$, is a permutation of Y^X, this is easy to see. Since for $\pi, \rho \in H$:

$$\widehat{\pi\rho} = \hat{\pi}\hat{\rho},$$

the elements $\hat{\pi}$ form a subgroup of the symmetric group S_{Y^X} on Y^X, which is homomorphic to H. This subgroup is denoted by E^H:

$$E^H = \{\hat{\pi} \mid \hat{\pi} \in H\} \leq S_{Y^X}.$$

If Y consists of more than one element, then E^H is even isomorphic to H.

In terms of this permutation group E^H, the equivalence class of $f \in Y^X$ is just the orbit of E^H which contains f. Hence by Burnside's lemma, which gives the number of orbits of a permutation group as the sum over the fixed points of its elements divided by the order of the group, the number of orbits of E^H, i.e. the number of equivalence classes of functions is equal to

1.1 $$\frac{1}{|E^H|} \sum_{\hat{\pi} \in E^H} a_1(\hat{\pi}),$$

if $a_1(\hat{\pi})$ denotes the number of functions fixed under $\hat{\pi}$. By the homomorphism theorem of group theory we see that 1.1 is equal to

1.2 $$\frac{1}{|H|} \sum_{\pi \in H} a_1(\hat{\pi}),$$

and it is not difficult to see that

$$a_1(\hat{\pi}) = |Y|^{c(\pi)},$$

if

$$c(\pi) = \sum_{i=1}^{|X|} a_1(\pi)$$

denotes the number of cyclic factors of π (recall from part I that $a_i(\pi)$ denotes the number of cyclic factors of π which are of length i). We thus end up with the result that

1.3 $$\frac{1}{|H|} \sum_{\pi \in H} |Y|^{c(\pi)}$$

is the desired number of orbits.

2. Formulation in terms of representation theory.

In the preceding section we saw that our problem amounts to a description of the orbits of the permutation group E^H on Y^X. We can formulate this also in terms of representation theory if we consider the corresponding permutation representation. This is a little bit more complicated but it has the advantage that it comprises more of algebraic structure since we are then dealing with a permutation group which acts on a vector space. It allows then to apply all what we know about representations of finite groups.

The permutation representation corresponding to the action of E^H on Y^X is defined as follows. We take the free vector space over the field $\mathbb{C}$ of complex numbers which has the set Y^X as basis, i.e. we consider the set of formal expressions

$$\sum_{f\in Y^X} c_f f,$$

where the coefficients c_f are complex numbers, where two such expressions $\sum c_f f$ and $\sum d_f f$ are equal if and only if for each $f \in Y^X$ we have $c_f = d_f$, where

$$\sum_f c_f f + \sum_f d_f f = \sum_f (c_f + d_f) f,$$

and, for $c \in \mathbb{C}$,

$$c \sum c_f f = \sum_f (c c_f) f.$$

The elements $f \in Y^X$ form a basis of this vector space V (which is of dimension $|Y^X| = |Y|^{|X|}$), so that a linear transformation of V is uniquely determined by giving the images of the elements $f \in Y^X$. The linear mapping of V onto itself which is associated with π is the mapping $D(\pi)$, defined by

2.1 $$D(\pi) : f \longmapsto f \circ \pi^{-1},$$

i.e. the element f of the basis of V is mapped onto the basis vector $f \circ \pi^{-1}$. From the preceding section we know that we have for the character χ^D of this representation:

2.2 $$\chi^D(\pi) = |Y|^{c(\pi)}.$$

An important fact which we can cite from representation theory now is that we can decompose the representation space V into a direct sum of irreducible invariant subspaces which are (up to isomorphism) uniquely determined. These are called the irreducible constituents of V. The equivalence classes $[f]_\sim$ of Y^X, i.e. the subsets

$$[f]_\sim = \{f_1 \mid f_1 \in Y^X,\ f_1 \sim f\}$$

of the basis Y^X of V generate subspaces of V:

2.3 $$V_f = \langle [f]_\sim \rangle .$$

Since each $[f]_\sim$ is mapped onto itself under each $D(\pi)$, $\pi \in H$, the subspaces V_f are invariant. V is a direct sum of these subspaces:

2.4 $$V = \bigoplus_{f \in Y^X} V_f = \bigoplus_{f \in Y^X} \langle [f]_\sim \rangle .$$

But these subspaces V_f are in general reducible, so that this decomposition 2.4 is still not fine enough. But already this decomposition is quite helpful. For it is easy to see that each one of these subspaces contains the identity representation I of H (which has character $\chi^I(\pi) = 1$, for each $\pi \in H$) exactly once. Hence the number of different subspaces V_f, i.e. the number of different equivalence classes $[f]_\sim$ is equal to the multiplicity (D,I) of I in D. But this multiplicity (D,I) is just the inner product of the characters:

2.5 $$(D,I) = \frac{1}{|H|} \sum_{\pi \in H} \chi^D(\pi)\chi^I(\pi^{-1}) = \frac{1}{|H|} \sum_{\pi \in H} \chi^D(\pi) \cdot 1 = \frac{1}{|H|} \sum_{\pi \in H} |Y|^{c(\pi)} .$$

This gives 1.3 again.

3. The irreducible constituents of D

We start considering the special case when H is equal to the symmetric group on X:

$$H = S_X$$

In this particular case the decomposition of D into its irreducible constituents is known. (In fact, this representation D of S_X occurs in general representation theory in a connection which is very important for applications, namely the decomposition of Kronecker powers of representations into symmetrized products.)

It is well known how we can associate the irreducible representations of S_X with ordered partitions $\alpha = (\alpha_1, \dots, \alpha_h)$ of $|X|$ in such a way that representations associated with different partitions are inequivalent. We denote the representation associated with α by $[\alpha]$ as usual. Then it can be shown that the following holds:

3.1 (i) $[\alpha]$, where $\alpha = (\alpha_1, \dots, \alpha_h)$ occurs under the irreducible constituents of D if and only if $h \leq |Y|$.

(ii) The multiplicity $f^{\langle\alpha\rangle}$ of $[\alpha]$ in D can be evaluated as follows: If again $\alpha = (\alpha_1, \dots, \alpha_h)$, then

$$f^{\langle\alpha\rangle} = \frac{f^{\alpha}}{n!} \prod_{\substack{1 \leq i \leq h \\ 1 \leq j \leq \alpha_i}} (m+j-i),$$

where f^{α} denotes the dimension of $[\alpha]$.

In the case when H is a proper subgroup of S_X, we obtain the decomposition of the representation D of H into its irreducible constituents from 3.1, if we know the multiplicities $([\alpha]\downarrow H,F)$ of the irreducible representations F of H in the restrictions $[\alpha]\downarrow H$ of the representations $[\alpha]$ of S_X to the subgroup H of S_X. These multiplicities can be obtained from the character tables of H and S_X. We then obtain for the multiplicity of F in D:

3.2 $$(D,F) = \sum_{\alpha \vdash n} f^{\langle\alpha\rangle}([\alpha]\downarrow H,F)$$

In particular,

3.3 $$(D,I) = \sum_{\alpha \vdash n} f^{\langle\alpha\rangle}([\alpha]\downarrow H,I).$$

In order to evaluate $([\alpha]\downarrow H,I)$ we may apply Frobenius' reciprocity theorem which says that this multiplicity is the same as the multiplicity of $[\alpha]$ in $IH\uparrow S_X$, i.e. representation of S_X induced from the identity representation IH of H:

3.4 $$([\alpha]\downarrow H,I) = (IH\uparrow S_X, [\alpha]).$$

Let us consider a numerical example.

It is well known that the character table of S_4 is as follows:

Class type:	1^4	$1^2 2$	$1\ 3$	4	2^2
Order:	1	6	8	6	3
[4]	1	1	1	1	1
[3,1]	3	1	0	-1	-1
$[2^2]$	2	0	-1	0	2
$[2,1^2]$	3	-1	0	1	-1
$[1^4]$	1	-1	1	-1	1

The dihedral group D_4, the symmetry group of the square, has the following character table:

Class type:	1^4	$1^2 2$	2^2	2^2	4
Order:	1	2	1	2	2
F_1	1	1	1	1	1
F_2	1	1	1	-1	-1
F_3	1	-1	1	1	-1
F_4	1	-1	1	-1	1
F_5	2	0	-2	0	0

These two character tables yield for the multiplicities $([\alpha]\downarrow D_4, F_i)$:

$([\alpha]\downarrow D_4, F_i)$	F_1	F_2	F_3	F_4	F_5
[4]	1	0	0	0	0
[3,1]	0	1	0	0	1
$[2^2]$	1	0	1	0	0
$[2,1^2]$	0	0	0	1	1
$[1^4]$	0	0	1	0	0

The $f^{\langle\alpha\rangle}$ turn out to be (we take m=3):

$[\alpha]$	$f^{\langle\alpha\rangle}$
[4]	15
[3,1]	15
$[2^2]$	6
$[2,1^2]$	3
$[1^4]$	0

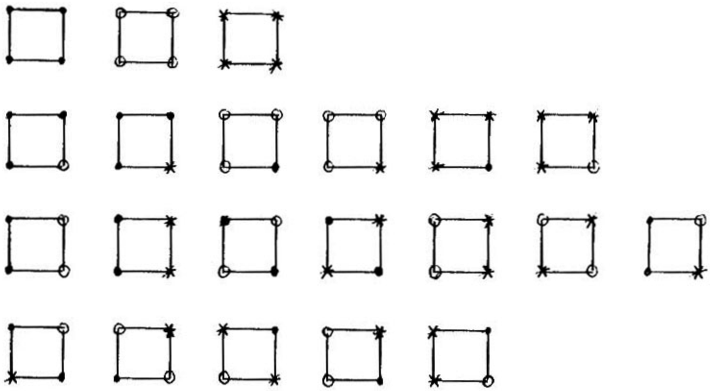
This shows that the decomposition of the representation D of S_4 into its irreducible constituents is just

$$D = 15[4] + 15[3,1] + 6[2^2] + 3[2,1^2],$$

while the decomposition of its restriction to the subgroup D_4 is

$$D\downarrow D_4 = 21\cdot F_1 + 15\cdot F_2 + 6F_3 + 3F_4 + 18F_5$$

The multiplicity 21 of F_1 shows that there are exactly 21 equivalence classes of mappings from $\{1,2,3,4\}$ into $\{1,2,3\}$ with respect to D_4 as symmetry group. Let us illustrate them by corresponding colourings of the square by the three colours • , ∘ and ∗:



(It is clear that the resulting number 21 can be obtained much quicker as multiplicity of F_1 in the restriction $D{\downarrow}H$ which has character

$$\chi^D(\pi) = 3^{c(\pi)}$$

as it is mentioned above. But we are interested in the complete decomposition of D at the moment.)

4. The introduction of S-functions

The reader knows that the enumeration theory yields stronger results than the number of equivalence classes only. For the famous theorem of Pólya says that the number of equivalence classes of kind $(k_1, \ldots, k_{|Y|})$ (i.e. of functions which take k_i-times the i-th element of Y, $1 \leq i \leq |Y|$) is just the coefficient of

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

in the polynomial

$$Z(H \mid y_1 + \ldots + y_{|Y|}). \tag{4.1}$$

This polynomial 4.1 arises from the cycle-index polynomial

$$Z(H) = \frac{1}{|H|} \sum_{\pi \in H} x_1^{a_1(\pi)} \cdots x_{|X|}^{a_{|X|}(\pi)} \tag{4.2}$$

by substituting

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

for x_i in $Z(H)$.

In order to show how 4.1 can be obtained from a representation theoretical consideration, we define a generalization of 4.2.

If F denotes a representation of H which has character χ^F, then we put

4.3 $$Z(H,F) = \frac{1}{|H|}\sum_{\pi\in H}\chi^F(\pi)\, x_1^{a_1(\pi)} \dots x_{|X|}^{a_{|X|}(\pi)} .$$

A particular representation of S_X is the representation $IH\uparrow S_X$ which is induced from the identity representation IH of H which was already mentioned above. It is not difficult to show that the following holds:

4.4 $$\begin{aligned} Z(H) &= Z(S_X,\ IH\uparrow S_X) \\ &= Z(S_X,\ \sum_{\alpha\vdash n}(IH\uparrow S_X,\ [\alpha])[\alpha]) \\ &= \sum_{\alpha\vdash n}(IH\uparrow S_X,\ [\alpha])\ Z\ (S_X,\ [\alpha]) \end{aligned}$$

The polynomial $Z(S_X,[\alpha])$, which satisfies

$$Z(S_X,[\alpha]) = \frac{1}{|X|!}\sum_{\pi\in S_X}\zeta^\alpha(\pi)(y_1^1 + \dots + y_{|Y|}^1)^{a_1(\pi)} \dots$$
$$\dots (y_1^{|X|} + \dots + y_{|Y|}^{|X|})^{a_{|X|}(\pi)}$$

is often denoted by $\{\alpha\}$:

$$\{\alpha\} = Z(S_X,[\alpha]).$$

These polynomials corresponding to partitions α are called <u>S-functions</u>.

This altogether yields the result

$$4.5 \quad Z(H \mid y_1 + \ldots + y_{|Y|}) = \sum_{\alpha \vdash |X|} (IH{\uparrow}S_X, [\alpha])\{\alpha\},$$

which shows that the generating function for our combinatorial problem is a sum of S-functions which can be obtained from the character table of S_X once we know the decomposition of $IH{\uparrow}S_X$ into its irreducible constituents. If we again consider $ID_4{\uparrow}S_4$ as in the preceding section, we already know

$$ID_4{\uparrow}S_4 = [4] + [2^2],$$

so that

$$Z(D_4 \mid y_1 + y_2 + y_3) = \{4\} + \{2^2\}$$

Let us remark that S-functions $\{\alpha\}$ occur in representation theory as polynomial functions which yield character values. For if $GL_{|Y|}$ denotes the group of all the non-singular matrices over the complex field which have $|Y|$ rows and columns and if $\alpha = (\alpha_1, \ldots, \alpha_h)$ is a partition of $|X|$ where $h \leq |Y|$, then $\{\alpha\}$ yields a certain irreducible character $\zeta^{\langle\alpha\rangle}$ of $GL_{|Y|}$ if we put for $g \in GL_{|Y|}$:

$$4.6 \qquad \zeta^{\langle\alpha\rangle}(g) = \{\alpha\}(\varepsilon_1, \ldots, \varepsilon_{|Y|}),$$

if $\varepsilon_1, \ldots, \varepsilon_{|Y|}$ are the eigenvalues of the matrix $g \in GL_{|Y|}$.

There are not many subgroups H of symmetric groups S_X where $IH\uparrow S_X$ is known explicitly. But for the alternating group $A_X \leq S_X$ we know for example that the irreducible constituents of $IA_X\uparrow S_X$ are just the identity representation and the alternating representation. Since $[n]$ is the identity representation and $[1^n]$ the alternating representation of S_n, we obtain

4.7 (i) $Z(S_n \mid y_1 + \dots + y_{|X|}) = \{n\}$,

(ii) $Z(A_n \mid y_1 + \dots + y_{|Y|}) = \{n\} + \{1^n\}$.

Another prominent subgroup of S_n is the cyclic subgroup of order n, $C_n = \langle(1 \dots n)\rangle$, which is generated by the cycle $(1 \dots n)$. The representation $IC_n\uparrow S_n$ has the character $\chi^{IC_n\uparrow S_n}$ with value

4.8 $$\chi^{IC_n\uparrow S_n}(\pi) = \frac{n!}{n} \frac{|C(\pi) \cap C_n|}{|C(\pi)|},$$

where $C(\pi)$ denotes the conjugacy class of $\pi \in S_n$. $\pi \in S_n$ is contained in C_n, at most if π consits of n/i cycles of length i, i a divisor of n. In this case we have

$$|C(\pi) \cap C_n| = \varphi(i),$$

φ the Euler function, i.e.

$$\varphi(i) = |\{k \mid k \in \mathbb{N}, k \leq i, (k,i) = 1\}|,$$

where (k,i) denotes the greatest common divisor of k and i.

This gives for the multiplicity of $[\alpha]$ in $IC_n\uparrow S_n$:

$$4.9 \quad (IC_n\uparrow S_n,[\alpha]) = \frac{1}{n!}\sum_{\pi\in S_n}\zeta^{\alpha}(\pi^{-1})\chi^{IC_n\uparrow S_n}(\pi)$$

$$= \frac{1}{n}\sum_{\pi\in S_n}\zeta^{\alpha}(\pi^{-1})\ \frac{|C(\pi)\cap C_n|}{|C(\pi)|}$$

$$= \frac{1}{n}\sum_{i|n}\varphi(i)\ \zeta^{\alpha}_{(i^{n/i})}.$$

where $\zeta^{\alpha}_{(i^{n/i})}$ denotes the value of the character ζ^{α} of $[\alpha]$ at an element consisting of n/i cyclic factors of length i.

This altogether yields:

$$4.10 \quad Z(C_n|y_1+\ldots+y_{|Y|}) = \sum_{\alpha\vdash n}\left(\frac{1}{n}\sum_{i|n}\varphi(i)\zeta^{\alpha}_{(i^{n/i})}\right)\{\alpha\}.$$

$$= \frac{1}{n}\sum_{i|n}\varphi(i)\sum_{\alpha\vdash n}\zeta^{\alpha}_{(i^{n/i})}\{\alpha\}$$

A useful result on symmetric polynomials which may be applied now is

<u>4.11</u> If we abbreviate

$$s_i = y_1^i+\ldots+y^i_{|Y|}$$

(this symmetric polynomial is called <u>power sum symmetric function</u>), and put for a partition $\beta = (\beta_1,\ldots,\beta_k)$ of $|X|$

$$s_\beta = s_{\beta_1}\cdot s_{\beta_2}\ldots\cdot s_{\beta_k}$$

then

$$s_\beta = \sum_{\alpha \vdash n} \zeta_\beta^\alpha \{\alpha\},$$

where ζ_β^α denotes the character of $[\alpha]$ at an element with cycle decomposition $(\beta_1, \ldots, \beta_k)$ in S_X.

An application of 4.11 to 4.10 yields the well known result

4.12 $$Z(C_n | y_1 + \ldots + y_{|Y|}) = \frac{1}{n} \sum_{i|n} \varphi(i) s_i^{n/i}.$$

This result is of course well known and can be obtained also directly from the cycle structure of C_n. But I stressed the fact that it can be obtained via representation theoretical considerations since representation theory yields much more in particular if we consider situations which are more general than this Pólyatype situations as it will be shown in a subsequent part of this paper.

Let me conclude by giving a few references which contain more details on applications of representation theory to enumeration.

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