Enumeration by Stabilizer Class of Patterns with Local Restrictions

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Abstract

We consider patterns of colourings of G-sets where certain forbidden sub-colourings are excluded. An algorithm is developed for the calculation of inventories of patterns with a prescribed stabilizer class.

1 Introduction

The theory of pattern enumeration is concerned with a finite group G acting as the group of symmetries of a set X, a set of colours C, and the action of G on the set C^X of colourings of X. By a *pattern* we mean the G-orbit of a colouring.

Williamson [6] used a combination of the inclusion - exclusion rule with Redfield/Pólya theory to enumerate patterns of colourings which do not contain colourings of specified subsets of X using chosen subsets of C. The aim of this note is to enumerate the subset of these patterns which are stabilized by a chosen conjugacy class of subgroups of G.

We use two examples to illustrate the main features of the method. Firstly we discuss a particular example used by Williamson which involves the enumeration of patterns of 8-bead necklaces that do not include particular sub-colourings called *a-rooted trees*. A second example is taken from the counting of isomers in chemical enumeration. We consider colourings

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of the 8 vertices of a trigonal dodecahedron in which the vertices are of two types, 4-valent and 5-valent, and such that adjacent vertices have different colours. The additional feature here is that excluded colourings may be constructed in different ways from sets of forbidden sub-colourings.

We end by writing down a general algorithm for enumerating inventories of patterns which exclude an arbitrary number of sub-colourings that are specified using an arbitrary partition of the set of colours.

2 Pattern enumeration

We first recall some of our notation and results from [4] and [5]. Enumeration by stabilizer class using tables of marks is also discussed in detail in Chapter 3 of [1].

Denote by $\mathcal{L}_G$ and $\mathcal{P}_G$ the subgroup lattice and the poset of conjugacy classes $[H]$ of subgroups of a group G. Let $\mathcal{A}$ be a commutative algebra over the rationals. The incidence algebra $\mathcal{A}IA(L_G)$ has a subalgebra $\mathcal{A}CA(L_G)$ of *conjugacy functions* satisfying

$$f(H,K) = f(g^{-1}Hg, g^{-1}Kg) \text{ for all } H,K \leq G \text{ and } g \in G.$$

There is an algebra homomorphism from $\mathcal{A}CA(\mathcal{L}_G)$ to $\mathcal{A}IA(\mathcal{P}_G)$ which maps f to $\check{f}$ where

$$\check{f}([H],[K]) = \sum_{K' \in K} f(H,K').$$

Let ζ be the zeta function on $\mathcal{L}_G$ with inverse the Möbius function μ, and let γ be the conjugacy diagonal function defined by $\gamma(K) = |G| \,/\, |K|\,|[K]|$. The *mark* function $\phi \in \mathcal{A}IA(\mathcal{P}_G)$, where $\phi([H],[K])$ is the number of left cosets in (G/K) fixed under left multiplication by H, has a factorisation $\phi = \check{\zeta}\gamma$. When a total ordering of the classes $[K]$ has been chosen, compatible with the partial order on $\mathcal{P}_G$, the marks form an upper triangular matrix $M(\phi)$, known as the *table of marks* of G, whose inverse is the *Burnside matrix* $M(\phi^{-1})$.

Given a diagonal conjugacy function Δ on $\mathcal{L}_G$ we obtain $\check{\tau}$ from α and τ where

$$\alpha = \mu\Delta\zeta, \quad \tau = \gamma^{-1}\alpha\gamma, \quad \check{\tau} = \phi^{-1}\Delta\phi. \tag{1}$$

The values $\alpha(H,K)$ may be calculated successively, working downwards from K using the intervals $[H,K]$, by the formulae

$$\alpha(K,K) = \Delta(K), \qquad \sum_{H \leq J \leq K} \alpha(H,J) \;=\; 0 \text{ when } H \neq K. \tag{2}$$

In the case $K = G$,

$$\check{\tau}([H],[G]) = \alpha(H,G)/\gamma(H). \tag{3}$$

We now summarise the basic ingredients of generalised Redfield/Pólya enumeration (see, for example, [1], Chapter 2, or [5], Section 5). Let G be a subgroup of the symmetric group S_n

and let $\mathcal{A} = \Lambda_\ell \otimes \mathbb{Q}$ where Λ_ℓ is the ring of symmetric polynomials in a set of indeterminates $\Xi_\ell = \{\xi_1, \xi_2, \ldots, \xi_\ell\}$, generated by the power sums $p_d = \sum_{i=1}^{\ell} \xi_i^d$. When we wish to consider two sorts of indeterminates, we write $\Xi_\ell = \{\eta_1, \ldots, \eta_j, \theta_1, \ldots, \theta_k\}$, $j + k = \ell$, and we denote by q_d, r_d the power sums in η_i, θ_i respectively, so that $p_d = q_d + r_d$ for all $d \geq 1$.

Let V be a G-set and $w : V \to \mathcal{A}$ a weight function. The weight of a subset $U \subseteq V$ is defined to be $w(U) = \sum_{u \in U} w(u)$. For $g \in G$ and $H \leq G$ we denote the weights of the fixed point subsets $\mathrm{Fix}_V(g)$ and $\mathrm{Fix}_V(H)$ by $w(V, g)$ and $w(V, H)$ respectively. If Ω is a transversal for the set of orbits V/G and w is constant on each orbit, the *inventory* of V is $w(\Omega)$. Each $g \in G$ determines a partition $\pi_g = (n^{m_n} \ldots 2^{m_2} 1^{m_1})$ of n, in which the parts are the lengths of the disjoint cycles, and hence a symmetric function

$$p_g \ = \ p_n^{m_n} \ldots p_2^{m_2} p_1^{m_1} \ = \ w(V, g) \ \in \ \Lambda_\ell,$$

the combined weight of all the elements fixed by g. The Cauchy-Frobenius Lemma states that

$$w(\Omega) = \frac{1}{|G|} \sum_{g \in G} p_g.$$

Similarly, each subgroup H of G determines a partition $\pi_H = (\pi_1, \pi_2, \ldots, \pi_h) \vdash n$, in which the parts are the lengths of the orbits, and hence a symmetric function

$$p_H = p_{\pi_1} p_{\pi_2} \ldots p_{\pi_h} = w(V, H) \in \Lambda_\ell,$$

the weight of all the elements fixed by H.

Defining $\Delta_p \in \mathcal{A}CA(\mathcal{L}_G)$, $H \mapsto p_H$, we obtain by (1)

$$\check{\tau}_p \ = \ \phi^{-1} \Delta_p \phi \ \in \ \mathcal{A}IA(\mathcal{P}_G).$$

(The matrix $M(\check{\tau}_p)$ is the transition matrix between β-operations and λ-operations of degree n in a β-ring (see [5], Corollary 5.2).)

Let $V_{[H]}$ be the subset of V whose elements have stabilizer class $[H]$ and let $\Omega_{[H]}$ be a transversal for $V_{[H]}/G$. The $[H]$-inventories $w(\Omega_{[H]})$ of V may be obtained by multiplying the vector whose elements are the values of Δ_p by the Burnside matrix ([1], Section 3.3). Since this vector forms the final column of the matrix $M(\Delta\phi)$, these inventories are the entries $\check{\tau}_p([H], [G])$ in the last column of $M(\check{\tau}_p)$.

Now let X be an n-element G-set, let $C = \{c_1, c_2, \ldots, c_\ell\}$ be a set of colours and let $w_C : C \to \mathcal{A}, c_i \mapsto \xi_i$ be a weight function on the colours. The set $V = C^X$ of colourings of X has weight function

$$w : V \to \mathcal{A}, \ \ \chi \mapsto \prod_{x \in X} w_C(\chi(x)).$$

Pólya's fundamental theorem states that the inventory of V is the cycle index

$$\mathrm{Cyc}(G;\ p_1, p_2, \ldots, p_n) = \frac{1}{|G|} \sum_{g \in G} p_g \ \in \ \mathcal{A}.$$

3 Williamson's example

Given a set $X = \{1, 2, \ldots, 8\}$ of 8 beads on a circular necklace, consider the set $V_0 = C^X$ of colourings of the beads using a set of colours $C = A \cup B$, $A = \{a_1, a_2, \ldots, a_j\}$, $B = \{b_1, b_2, \ldots, b_k\}$, $A \cap B = \emptyset$. The dihedral group D_{16} acts as the group of symmetries of the uncoloured necklace and has cycle index, expressed as a polynomial in $j = |A|$, $k = |B|$:

$$\mathrm{Cyc}(D_{16}, \{j,k\}) = j^8 + j^7k + 4j^6k^2 + 5j^5k^3 + 8j^4k^4 + 5j^3k^5 + 4j^2k^6 + jk^7 + k^8.$$

There are 30 patterns when $j = k = 1$; 987 patterns when $j = 2$ and $k = 1$; and 7680 patterns when $j = k = 2$.

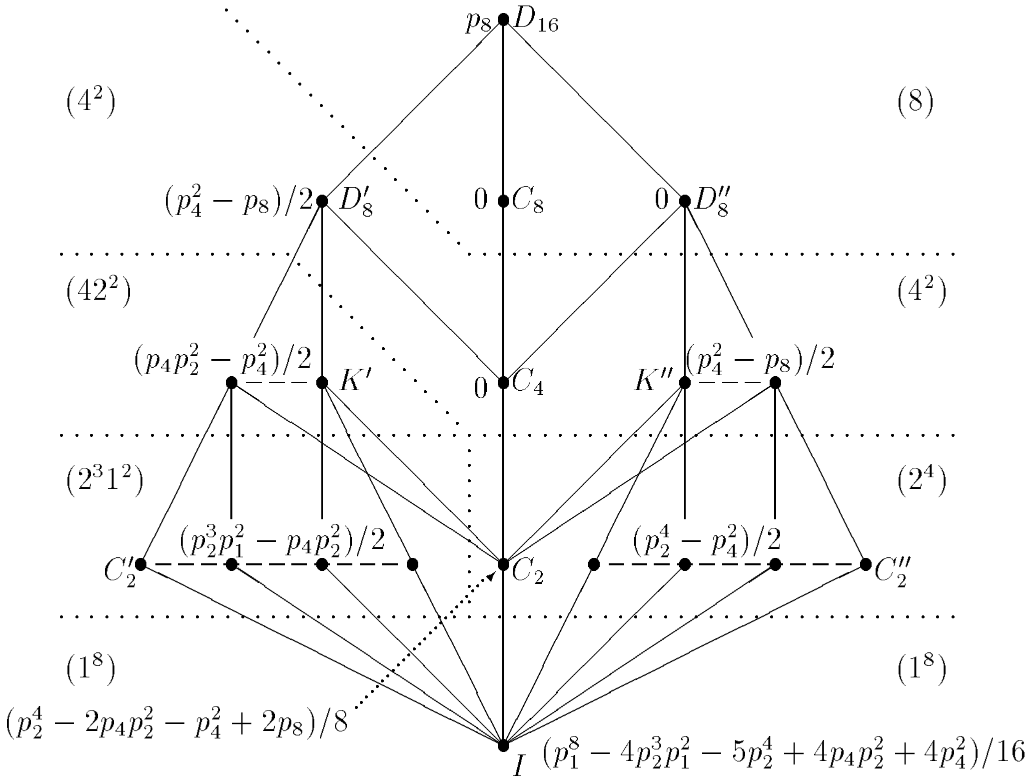


Figure 1: Subgroup Lattice of D_{16} and values $\check{\tau}_p([H], [D_{16}])$.

A Hasse diagram for the subgroup lattice of D_{16} is shown in Figure 1, where horizontal dashed lines join the subgroups in a conjugacy class $[H]$. The class $[C_2']$, (resp. $[C_2'']$) contains those reflections whose axis does (resp. does not) pass through a pair of beads. Dotted lines partition the lattice of D_{16} into subposets in which the subgroups have constant orbit type $\pi_H \vdash 8$. The poset formed by these regions is isomorphic to the subposet $\{\pi_H | H \leq D_{16}\}$ of the poset of all partitions of 8. Values $\check{\tau}_p([H], [D_{16}])$ are shown for each conjugacy class $[H]$. Note that $\check{\tau}_p([H], [D_{16}) = 0$ when the subgroups in $[H]$ are *not* maximal in the subposet of type π_H.

Summing over all subgroup classes, we obtain the cycle index:

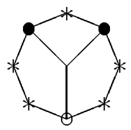
$$\sum_{H \leq D_{16}} \check{\tau}_p([H], [D_{16}]) \ = \ \mathrm{Cyc}(D_{16};\ p_1, \ldots, p_8) \ = \ \frac{1}{16}(p_1^8 + 4p_2^3 p_1^2 + 5p_2^4 + 2p_4^2 + 4p_8).$$

When Δ is an arbitrary diagonal function, constant on these subposets, the non-zero values of $\check{\tau}([H], [D_{16}])$ are given in Table 1.

H	$\check{\tau}([H], [D_{16}])$
D_{16}	$\Delta(D_{16})$
D_8'	$(\Delta(D_8') - \Delta(D_{16}))/2$
K''	$(\Delta(K'') - \Delta(D_{16}))/2$
K'	$(\Delta(K') - \Delta(D_8'))/2$
C_2''	$(\Delta(C_2'') - \Delta(K''))/2$
C_2'	$(\Delta(C_2') - \Delta(K'))/2$
C_2	$(\Delta(C_2) - 2\Delta(K') - 2\Delta(K'') + \Delta(D_8') + 2\Delta(D_{16}))/8$
I	$(\Delta(I) - \Delta(C_2) - 4\Delta(C_2') - 4\Delta(C_2'') + 4\Delta(K') + 4\Delta(K''))/16$

Table 1: Values of $\check{\tau}$ for arbitrary Δ.

Williamson's problem was to determine the number of patterns which do *not* contain an a-rooted tree, namely a coloured subpattern of the form marked in Figure 2.



$\circ \in A, \quad \bullet \in B, \quad * \in C = A \cup B$

Figure 2: A necklace containing an a-rooted tree.

In the case $\ell = 2$, $\Xi = \{\eta, \theta\}$, rewriting the $\check{\tau}_p([H], [D_{16}])$ we obtain symmetric functions in η and θ as listed in Table 2. The 30 monomials correspond to the 30 colourings of the necklace with the set $\{a, b\}$. Just 13 of these have no a-rooted tree ([6], Figure 4).

Let $P = \{P_1, P_2, \ldots, P_8\}$ be the set of properties such that $\chi \in V_0$ satisfies P_i if χ contains an a-rooted tree with bead i as root. For $Q \subseteq P$ let

$$V_Q = \{\chi \in V_0 \mid \chi \text{ satisfies } P_i \text{ for all } P_i \in Q\}.$$

(8)	D_{16}	$\eta^8+\theta^8$
(4^2)	D_8'	$\eta^4\theta^4$
(4^2)	K''	$\eta^4\theta^4$
(42^2)	K'	$\eta^6\theta^2+\eta^2\theta^6$
(2^4)	C_2''	$2(\eta^6\theta^2+\eta^2\theta^6)+2\eta^4\theta^4$
(2^31^2)	C_2'	$(\eta^7\theta+\eta\theta^7)+(\eta^6\theta^2+\eta^2\theta^6)+3(\eta^5\theta^3+\eta^3\theta^5)+2\eta^4\theta^4$
(1^8)	I	$2(\eta^5\theta^3+\eta^3\theta^5)+2\eta^4\theta^4$

Table 2: Non-zero values of $\check{\tau}_p([H],[D_{16}])$ when $\ell=2$ (30 terms).

We represent the elements of V_Q by colourings having a *marked* a-rooted tree at each bead i for which $P_i \in Q$. If V_f is the set of colourings with *no* a-rooted tree then, using the principle of inclusion-exclusion, we define $\Delta_f \in \mathcal{A}CA(\mathcal{L}_G)$ by

$$\Delta_f(H) \;=\; w(V_f,H) \;=\; \sum_{Q\subseteq P}(-1)^{|Q|}\,w(V_Q,H). \tag{4}$$

If a colouring χ contains e a-rooted trees, then χ belongs to 2^e of the subsets V_Q and, if fixed by H, contributes $(1-1)^e=0$ to the sum (4). Only 47 of the 256 subsets V_Q are non-empty. For example, $V_{\{P_1,P_4\}}=\emptyset$ since properties P_1 *and* P_4 require beads 1 and 4 to be coloured with both A and B.

The first stage of the solution is to produce a complete set of *marked template patterns* T_t containing all possible arrangements of one or more a-rooted trees, modulo the group action. Such templates may be considered as patterns using $\{a,b,c\}$ as the set of colours: beads in the marked trees are coloured a (for the root) or b, the remaining beads are coloured c. In simple cases the templates can be found by inspection. In general, Williamson's multilinear techniques ([6], Section 2) may be used to construct them.

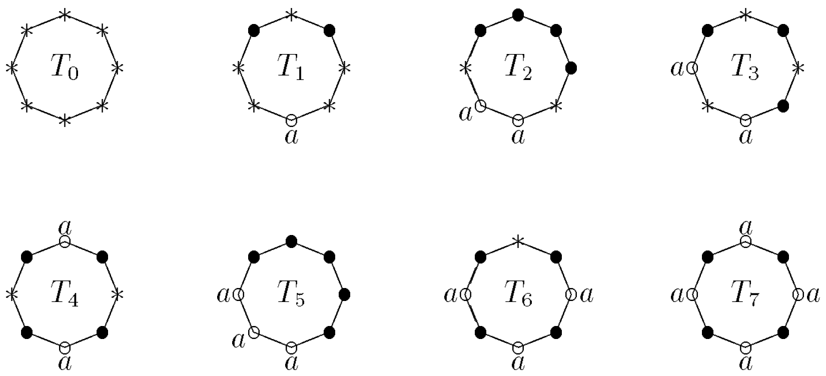


Figure 3: The 8 template patterns T_t.

The 8 templates for our example are shown in Figure 3, where $\circ, \bullet, *$ denote vertices coloured a, b, c respectively. Since an a-rooted tree is uniquely determined by the location of its root, we mark each tree by placing an a next to the root bead. Denoting by ν_t the number of a-rooted trees in T_t, we have $\nu_0 = 0,\ \nu_1 = 1,\ \nu_2 = \nu_3 = \nu_4 = 2,\ \nu_5 = \nu_6 = 3$ and $\nu_7 = 4$.

The stabilizer classes for these templates are given in Table 3.

Template	T_0	T_1	T_2	T_3	T_4	T_5	T_6	T_7
Size of orbit	1	8	8	8	4	8	8	2
Stabilizer class	D_{16}	C_2'	C_2''	C_2'	K'	C_2'	C_2'	D_8'

Table 3: Stabilizers of the templates.

For ψ a *template colouring* in T_t, partition X into subsets $X_{\psi a}, X_{\psi b}, X_{\psi c}$ of beads coloured a, b, c respectively. A *marked colouring* of type T_t is obtained by recolouring the beads in $X_{\psi a}, X_{\psi b}, X_{\psi c}$ with colours from A, B, C respectively. If V_t denotes the set of marked colourings of type T_t then

$$|V_t| \;=\; |T_t|\, j^{|X_{\psi a}|}\, k^{|X_{\psi b}|}\, \ell^{|X_{\psi c}|}.$$

Since these template colourings include exactly the 47 non-empty V_Q, equation (4) may be rewritten as

$$\Delta_f(H) = \sum_{t=0}^{7} (-1)^{\nu_t}\ w(V_t, H). \tag{5}$$

In our example $|V_1| = 8jk^2\ell^5$ so when $j = k = 1$ there are 256 colourings with a single marked a-rooted tree. These colourings form 30 marked patterns and in Figure 4 we give a transversal for V_1/D_{16}, where $\sim$ indicates different markings of the same colouring. (It is a coincidence that V_0/D_{16} contains 30 patterns and V_1/D_{16} contains 30 marked patterns.)

Redefine the weight of each colour by

$$w_C : C \to \mathcal{A},\ a_i \mapsto \eta_i\ (1 \le i \le j),\ \ b_i \mapsto \theta_i\ (1 \le i \le k).$$

Let Ω_t be a transversal for the patterns V_t/D_{16}. For each class $[H]$ we require the $[H]$-inventory $w(\Omega_t)$ as a polynomial in the power sums p_d, q_d and r_d. Let $X/H = \{O_1, \ldots, O_h\}$ and let the orbit O_i contain d_i beads. Let V_ψ be the set of marked colourings of type T_t obtained from $\psi \in T_t$. Just as p_H is a product of power sums, one for each orbit, so the total weight $w(V_\psi, H)$ of colourings fixed by H is a product of h factors. If O_i contains a bead coloured a *and* a bead coloured b then $\mathrm{Fix}_{V_\psi}(H)$ is empty and $w(V_\psi, H) = 0$. If O_i contains only vertices in $X_{\psi c}$ then O_i contributes a factor $p_{d_i} = (q_{d_i} + r_{d_i})$. If O_i only contains vertices from $X_{\psi a} \cup X_{\psi c}$ (resp. $X_{\psi b} \cup X_{\psi c}$) then O_i contributes q_{d_i} (resp. r_{d_i}). We thus obtain $\Delta_t \in \mathcal{A}IA(\mathcal{P}_G)$ where

$$\Delta_t([H]) = w(V_t, H) = \sum_{\psi \in T_t} w(V_\psi, H) \in \mathcal{A}. \tag{6}$$

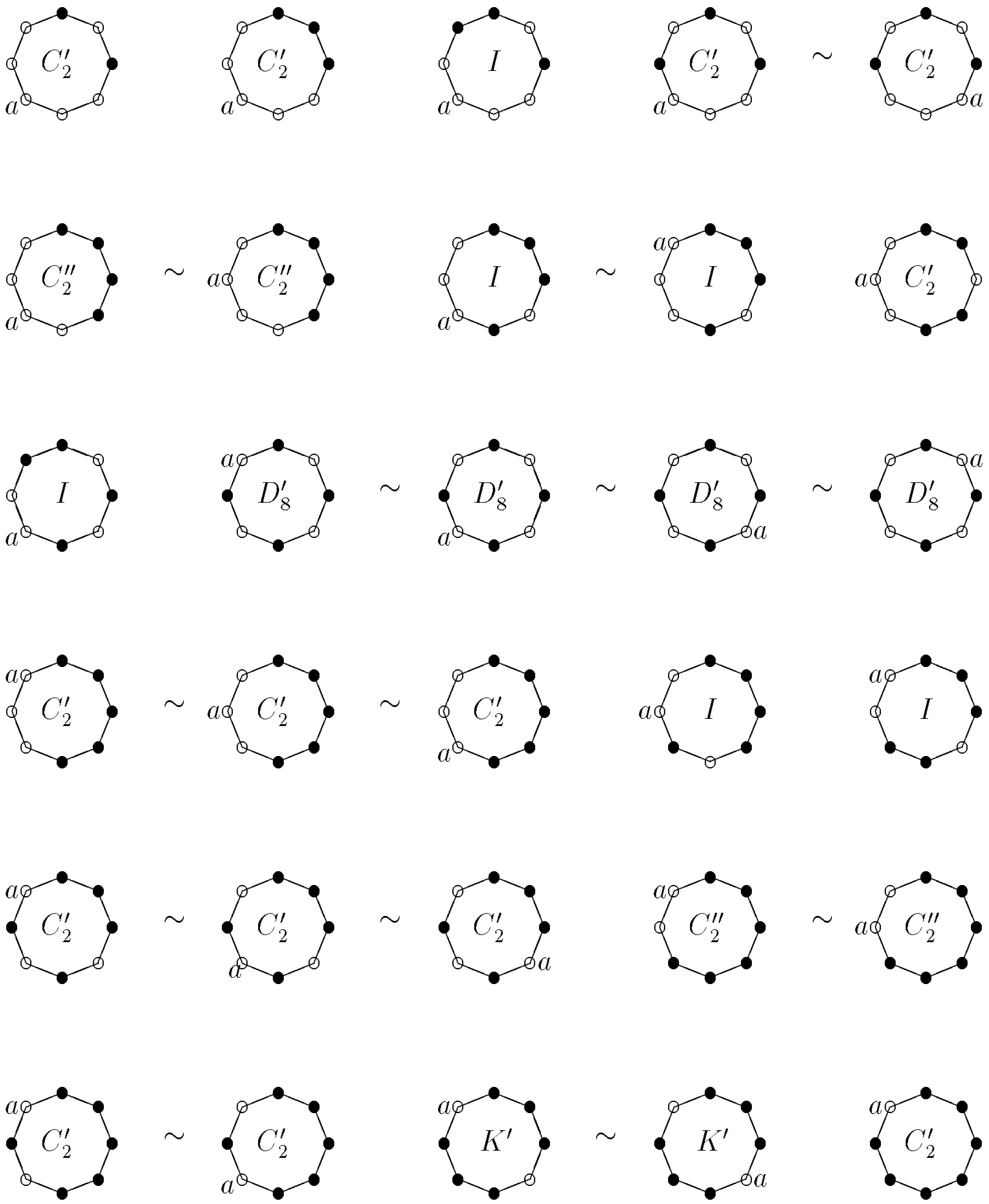


Figure 4: The 30 marked patterns of type T_1 and their stabilizer classes.

Reversing the order of summation in $\sum_{H'\in[H]}\sum_{\psi\in T_t} w(V_\psi, H')$, we obtain an alternative formula

$$\Delta_t([H]) = \frac{|T_t|}{|[H]|}\sum_{H'\in[H]} w(V_\psi, H'), \tag{7}$$

which is more convenient when the size of $[H]$ is small compared with that of T_t. Since Δ_t is a conjugacy function we may define $\check{\tau}_t = \phi^{-1}\Delta_t\phi$ and so $\check{\tau}_t([H],[D_{16}])$ is the inventory $w(\Omega_t)$.

Equations (4) and (5) define a conjugacy function Δ_f where $\Delta_f(H)$ is the total weight of the colourings which are free of a-rooted trees. The corresponding $\check{\tau}_f$ is given by a similar inclusion-exclusion formula:

$$\check{\tau}_f = \phi^{-1}\Delta_f\phi = \phi^{-1}\sum_{t=0}^{7}(-1)^{\nu_t}\Delta_t\phi = \sum_{t=0}^{7}(-1)^{\nu_t}\phi^{-1}\Delta_t\phi = \sum_{t=0}^{7}(-1)^{\nu_t}\check{\tau}_t.$$

and $w(\Omega_{f,[H]}) = \check{\tau}_f([H],[D_{16}])$ where Ω_f is a transversal for patterns with no a-rooted tree.

H	$\Delta_f(H)$
D_{16}, D_8'', C_8	p_8
D_8', C_4	$p_4^2 - 2q_4r_4$
K''	p_4^2
K'	$p_4p_2^2 - 2p_2q_2r_4 + q_2^2r_4 - q_4r_2^2$
C_2''	$p_2^4 - 2p_2q_2r_2^2$
C_2'	$p_2^3p_1^2 - 2p_2^2p_1q_1r_2 - 2p_2p_1q_2r_2r_1 + p_2q_1^2r_2^2 - p_1^2q_2r_2^2 + 2p_1q_2q_1r_2^2$ $+2q_2q_1r_2^2r_1 + q_2^2r_2r_1^2 - q_2q_1^2r_2^2$
C_2	$p_2^4 - 4p_2q_2r_2^2 + 2q_2^2r_2^2$
I	$p_1^8 - 8p_1^5q_1r_1^2 + 12p_1^2q_1^2r_1^4 + 8p_1^3q_1^2r_1^3 - 8p_1q_1^3r_1^4 - 8q_1^3r_1^5 + 2q_1^4r_1^4$

Table 4: Weights of colourings with no a-rooted tree.

The values of Δ_f are given in Table 4 and may be substituted in Table 1 to give the $[H]$-inventories for Ω_f. The first four of these contain relatively few terms:

$$\begin{aligned}
\check{\tau}_f([D_{16}],[D_{16}]) &= p_8 = \Sigma\eta_1^8 + \Sigma\theta_1^8\\
\check{\tau}_f([D_8'],[D_{16}]) &= (p_4^2 - p_8)/2 - q_4r_4 = \Sigma\eta_1^4\eta_2^4 + \Sigma\theta_1^4\theta_2^4\\
\check{\tau}_f([K''],[D_{16}]) &= (p_4^2 - p_8)/2 = \Sigma\eta_1^4\eta_2^4 + \Sigma\eta_1^4\theta_1^4 + \Sigma\theta_1^4\theta_2^4\\
\check{\tau}_f([K'],[D_{16}]) &= q_4(q_2^2 - q_4)/2 + q_4q_2r_2 + r_4(r_2^2 - r_4)/2\\
&= \Sigma\eta_1^6\eta_2^2 + \Sigma\eta_1^4\eta_2^2\eta_3^2 + \Sigma\eta_1^6\theta_1^2 + \Sigma\eta_1^4\eta_2^2\theta_1^2 + \Sigma\theta_1^6\theta_2^2 + \Sigma\theta_1^4\theta_2^2\theta_3^2
\end{aligned}$$

4 The trigonal dodecahedron

In [2] and [3] Lloyd has applied Redfield/Pólya methods to the enumeration of chemical isomers. In this situation the G-set $X = \{1,\dots,8\}$ is a molecule whose elements are termed *sites*, and these sites are 'coloured' with *ligands* which are groupings of one or more atoms.

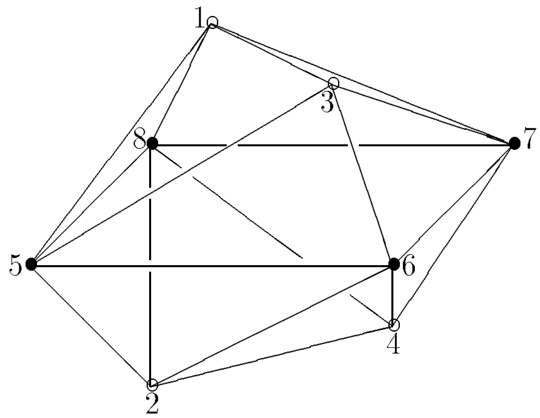


Figure 5: The trigonal dodecahedron.

There are chemical compounds which have eight ligands situated at the vertices of a trigonal dodecahedron (see Figure 5). The rotation group of the polyhedron contains three half-turns about mutually perpendicular axes, and the full rotation group is isomorphic to the dihedral group D_8 with elements

$$\begin{array}{cccc} (), & (13)(24)(57)(68), & (12)(34)(58)(67), & (14)(23)(56)(78), \\ (13)(68), & (24)(57), & (1432)(5876), & (1234)(5678). \end{array}$$

Since four of the sites are 4-valent and the remainder 5-valent, we colour $\{1,2,3,4\}$ with a set of ligands A and $\{5,6,7,8\}$ with a second set B. The appropriate cycle index is therefore

$$\mathrm{Cyc}(D_8, \{q_i, r_i \mid 1 \leq i \leq 4\}) = \frac{1}{8}(q_1^4 r_1^4 + 2q_2 q_1^2 r_2 r_1^2 + 3q_2^2 r_2^2 + 2q_4 r_4).$$

We suppose, as before, that $|A| = j$, $|B| = k$, and consider the enumeration of *non-adjacent colourings* χ : colourings such that no two adjacent sites contain the same ligand. In this example the set of properties is $P = \{P_{13}, P_{24}, P_{56}, P_{67}, P_{78}, P_{58}\}$ where χ satisfies P_{ih} if sites i and h contain the same ligand. First we restrict to the subset $P_A = \{P_{13}, P_{24}\}$, and call χ *A-adjacent* if $\chi(1) = \chi(3)$ or $\chi(2) = \chi(4)$. Then we apply the restriction to the square $\{5,6,7,8\}$, using $P_B = \{P_{56}, P_{67}, P_{78}, P_{58}\}$.

The only adjacent pairs of sites coloured with A are $\{1,3\}$ and $\{2,4\}$. Fix $a_i \in A$ and partition A as $\{a_i\} \cup \bar{A}_i$. There are only four types of marked template pattern, colouring X with $\{a_i, a_h, a, b\}$, as shown in Figure 6.

The inclusion-exclusion formula for the weight of the set A_f of colourings which are not A-adjacent is

$$\Delta_{A_f} = \Delta_0 - \sum_{i=1}^{j} \Delta_{1i} + \sum_{i=1}^{j} \Delta_{2i} + \sum_{i \neq h} \Delta_{2ih}.$$

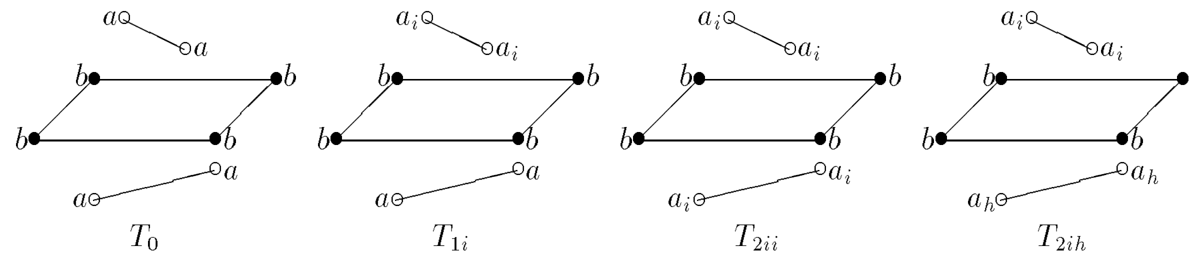


Figure 6: A-adjacent templates.

The individual $w(V_t, H)$ need not be symmetric functions, but become so under summation, as in

$$\sum_{i=1}^{j} w(V_{2ih}, K) = \sum_{i \neq h} \eta_i^2 \eta_h^2 r_2^2 = \frac{1}{2}(q_2^2 - q_4) r_2^2.$$

The only non-zero weights and $[H]$-enumerators are shown in Table 5.

$[H]$	$\Delta_{A_f}(H)$	$\check{\tau}_{A_f}([H],[D_{16}])$
C_2''	$(q_2^2 - q_4)r_2^2$	$(q_2^2 - q_4)r_2^2/2$
I	$(q_1^2 - q_2)^2 r_1^4$	$((q_1^2 - q_2)^2 r_1^4 - 2(q_2^2 - q_4)r_2^2)/8$

Table 5: Enumerators of non-A-adjacent patterns.

Now consider colourings in which adjacent sites among $\{5,6,7,8\}$ contain different ligands but with no restriction on $\{1,2,3,4\}$. The marked templates are shown in Figure 7.

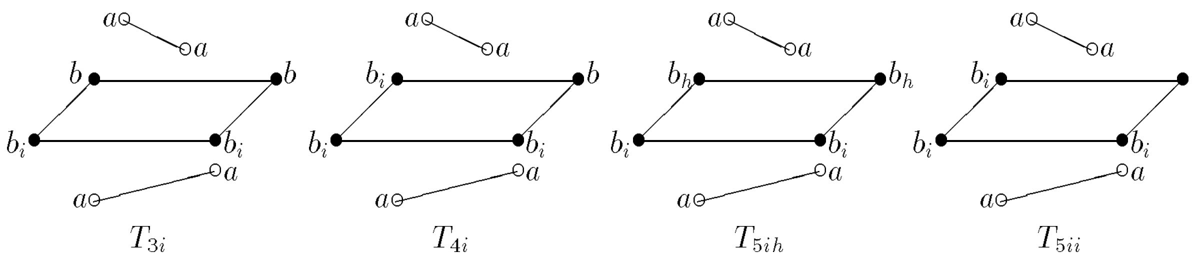


Figure 7: B-adjacent templates.

Because each site belongs to two adjacent pairs it is not the case, as in Williamson's example, that distinct $Q, Q' \subseteq P$ always give rise to different marked templates. In fact subsets

$$\{P_{56}, P_{78}\},\ \{P_{67}, P_{58}\},$$
$$\{P_{56}, P_{67}, P_{78}\},\ \{P_{56}, P_{67}, P_{58}\},\ \{P_{56}, P_{78}, P_{58}\},\ \{P_{67}, P_{78}, P_{58}\},$$
$$\{P_{56}, P_{67}, P_{78}, P_{58}\}$$

all give rise to marked templates T_{5ii}. Thus, when converting the general inclusion-exclusion formula (4) to a formula involving the Δ_t, the coefficient of Δ_{5ii} is $2 - 4 + 1 = -1$. The full formula is:

$$\Delta_{B_f} = \Delta_0 - \sum_{i=1}^{k} \Delta_{3i} + \sum_{i=1}^{k} \Delta_{4i} + \sum_{i \neq h}^{k} \Delta_{5ih} - \sum_{i=1}^{k} \Delta_{5ii}.$$

The only non-zero weights are

$$\begin{aligned} \Delta_{B_f}(K) = \Delta_{B_f}(C_2) &= q_2^2(r_2^2 - r_4), \\ \Delta_{B_f}(C_2''') &= q_2 q_1^2(r_2 r_1^2 - 2r_3 r_1 + r_4), \\ \Delta_{B_f}(I) &= q_1^4(r_1^4 - 4r_2 r_1^2 + 4r_3 r_1 + 2r_2^2 - 3r_4), \end{aligned}$$

where the subgroups in class $[C_2''']$ are generated by the reflections in the planes $1, 3, 6, 8$ and $2, 4, 5, 7$ and K is their join. The non-zero $[H]$-enumerators for B-adjacent free patterns are

$$\begin{aligned} \check{\tau}_{B_f}([K], [D_8]) &= \Delta_{B_f}(K)/2, \\ \check{\tau}_{B_f}([C_2'''], [D_8]) &= (\Delta_{B_f}(C_2''') - \Delta_{B_f}(K))/2, \\ \check{\tau}_{B_f}([I], [D_8]) &= (\Delta_{B_f}(I) - 2\Delta_{B_f}(C_2''') + \Delta_{B_f}(K))/8. \end{aligned}$$

In order to deal with non-adjacent colourings, we should need to consider all possible adjacencies, leading to a total of 20 marked templates. We omit the details.

5 The general algorithm

The following algorithm applies to an enumeration problem interpreted as the counting of patterns of valid colourings having a chosen stabilizer class $[H]$ in a group G. Colourings are invalid if they satisfy one or more of a set $P = \{P_1, P_2, \ldots, P_\lambda\}$ of forbidden properties. These properties may be expressed in terms of a partition $/A_1/A_2/\ldots/A_\kappa/$ of a set of colours C. If $A_i = \{a_{i1}, a_{i2}, \ldots, a_{ij_i}\}$ and $\sum_{i=1}^{\kappa} j_i = \ell$, take Ξ to be a set of ℓ indeterminates $\{\eta_{ih} \mid 1 \leq i \leq \kappa,\ 1 \leq h \leq j_i\}$ and let $w_c : C \to \mathcal{A},\ a_{ih} \mapsto \eta_{ih}$, be the corresponding weight function. Denote by q_{id} the power sum $\sum_{h=1}^{j_i} \eta_{ih}^d$ and by V_f the set of valid colourings.

Algorithm 5.1

1. Use Williamson's multilinear techniques to obtain a complete set of marked template patterns T_t coloured with a set of colours $\{c_1, c_2, \ldots, c_\kappa\}$.

2. For each template T_t and for each $[H] \leq [K] \leq [G]$ determine, using formulae (6) and (7), the weights $\Delta_t([K]) = w(V_t, K)$ as polynomials in the q_{id}.

3. Determine the total weight $\Delta_f([K])$ of colourings in V_f fixed by K by rewriting the inclusion-exclusion formula (4) for the λ properties as a signed sum of the $\Delta_t([K])$.

4. Calculate values of $\alpha_f = \mu\Delta_f\zeta$ and $\check{\tau}_f = \phi^{-1}\Delta_f\phi$ using equations (2) and (3), working down from $[G]$ over the interval $[\ [H],[G]\ ]$ of $\mathcal{P}_G$.

Theorem 5.2 *The polynomial $\check{\tau}_f([H],[G])$ is the $[H]$-inventory for patterns of valid colourings. When this polynomial is expressed as a polynomial in the indeterminates η_{ih}, the coefficient of $\prod \eta_{ih}^{d_{ih}}$ is the number of patterns in which colour a_{ih} is used d_{ih} times.*

References

[1] Kerber, A., Algebraic combinatorics via finite group actions, (Bibliographisches Institut Wissenschaftsverlag, Mannheim, 1991).

[2] Lloyd, E.K., Redfield's papers and their relevance to counting isomers and isomerizations, *Discrete Applied Math.* 19 (1988) 289-304.

[3] Lloyd, E.K., Marks of permutation groups and isomer enumeration, *J. Math. Chemistry* 11 (1992) 207-222.

[4] Morris, I. and Wensley, C.D. Adams operations and λ-operations in β-rings, *Discrete Math.* 50 (1984) 253-270.

[5] Morris, I. and Wensley, C.D., Cycle indices and subgroup lattices, *Discrete Math.* 118 (1993) 173-195.

[6] Williamson, S.G., The combinatorial analysis of patterns and the principle of inclusion-exclusion, *Discrete Math.* 1 (1972) 357-388.