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PÓLYA'S ENUMERATION THEOREM AND ITS APPLICATIONS

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Abstract

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1 Introduction

The number of colorings of the six faces of a cube fixed in space using n colors is easily found to be n^6 . Some of the colorings, however, are indistinguishable from one another if one allows the cube to be rotated in space. Enumerating the possible distinct n -colorings, taking rotations into consideration, becomes a non-trivial problem. Its solution can be found using group theory, particularly as an application of Burnside's lemma. Supposing further, that we wish to find the number of distinct colorings under rotations such that two faces have color A and four faces have color B , then Burnside's lemma alone is no longer sufficient. However, building on Burnside's lemma, Pólya's Enumeration Theorem (hereafter PET) proved to answer not only this question, but a whole class of related problems, which previously only had ad hoc solutions.[7]

In 1937, Hungarian mathematician George Pólya published a groundbreaking paper in combinatorial analysis describing a theorem which allowed a whole new class of enumeration problems to be solved. Entitled *Kombinatorische Anzahlbestimmungen für Gruppen, Graphen und chemische Verbindungen*, the paper ran over 100 pages, describing in depth PET and its applications in enumerating groups, graphs and chemical compounds. These applications brought Pólya's enumeration technique to the attention of the wider mathematical community, and many more applications have since been found. In 1960, it was discovered that an equivalent theorem to PET had been published by J. H. Redfield ten years before Pólya in 1927. Thus PET is sometimes known as the Pólya-Redfield Theorem.[7]

PET can be presented and explained using many different approaches.[7] In this thesis we follow mainly the approach of De Bruijn in [2] and Harary [4], as the generality of the theorem surfaces clearly. In its general form PET enumerates distinct functions between two non-empty sets X and Y , where X has a group of permutations G acting on its elements. The “colorings” then become equivalence classes induced in a natural way by G in Y^X , which are known as *configurations*. Each permutation group has associated with it what Pólya called the *cycle index*, which is a polynomial that is constructed based on the cycle structure of the group. PET then uses the cycle index associated with the group and produces a generating function which enumerates all possible configurations. Taking the cube coloring problem above, we have the group of rotational symmetries acting on the faces of the cube and the set of colors $\{A, B\}$. Using the appropriate cycle index, PET produces a generating function where the coefficient

of each $A^i B^j$ -term gives the number colorings with i faces of color A and j faces of color B . In this manner PET simultaneously enumerates all possible n -colorings.

After reviewing the required background knowledge, primarily in group theory, we state and prove Burnside's lemma. It is then applied to the cube coloring problem, which serves as a useful explanatory example throughout the thesis. Then, following discussions on the cycle index we proceed to explain and prove PET in detail. The thesis is concluded with several applications of PET. First it is applied to various coloring problems for necklaces and polyhedra. Further applications are given in the fields of number theory, graph theory, and chemistry. A general understanding of these topics is assumed.

2 Preliminary Concepts

Although in its essence PET is a combinatorial result, much of the machinery underlying it is algebraic in nature. This is evident from the fact that PET is based on Burnside's lemma, which is an important group theoretical result. Therefore, the focus of this chapter is on the underlying group theory. The basic ideas of equivalence relations and generating functions are also required in understanding PET, so they are briefly reviewed as well.

2.1 Group Theory

We begin by defining and reviewing some group theoretical concepts. In this section some results are stated without proof, as the proofs can be found in most standard books on algebra.

Definition 2.1. A **group**, denoted by $(G, *)$, is a non-empty set G equipped with a binary operation $*$ such that the following properties hold:

- (i) (Closure). If elements a and b are in G , then $a * b \in G$.
- (ii) (Associativity). If a, b , and c are elements in G , then $a * (b * c) = (a * b) * c$.
- (iii) (Identity element). There exists an element $e \in G$ such that $e * a = a = a * e$ for all $a \in G$. The element e is known as the identity element.
- (iv) (Inverse elements). If $a \in G$, then there exists an element $a^{-1} \in G$ such that $a * a^{-1} = e = a^{-1} * a$. The element a^{-1} is known as the inverse element of a .

The group $(G, *)$ is said to be **abelian** or **commutative**, if it also satisfies

- (v) (Commutativity). For all a and b in G , $a * b = b * a$.

The **order** of the group $(G, *)$ is the cardinality of the set G and it is denoted by $|(G, *)|$.

From this point on, if the group operation is clear from the context, the multiplicative notation will be used. In other words $a * b$ will simply be denoted by ab .

Definition 2.2. If G is a group, then any subset H of G which is also a group under the same operation as G is known as a **subgroup** of G . If H is a subgroup of G , one typically writes $H \leq G$.

Definition 2.3. If G is a group, $H \leq G$, and $g \in G$, then the **left coset** of H with respect to g is the set $gH = \{gh \mid h \in H\}$. The set of all left cosets of H in G is denoted by G/H . The number of left cosets of H in G is denoted by $[G : H]$ and is known as the **index** of H .

Theorem 2.4. (Lagrange's theorem) Let G be a group. If $H \leq G$, then

$$|G| = [G : H] \cdot |H|. \quad \square$$

Definition 2.5. Let A be a set, and $f : A \rightarrow A$ a bijective function. The function f is known as a **permutation of A** . If $S_A = \{f : A \rightarrow A \mid f \text{ is a permutation of } A\}$, and \circ represents the composition of functions, then (S_A, \circ) forms a group known as the **symmetric group of A** . A subgroup of (S_A, \circ) is known as a **group of permutations**. If $A = \{1, 2, \dots, n\}$, the symmetric group of A is denoted by S_n .

It is standard to represent a permutation $\sigma \in S_n$ in one of two ways. The first notation is to list the elements $1, 2, \dots, n$ in parentheses with their image under the permutation σ beneath them as follows¹:

$$\sigma = \begin{pmatrix} 1 & 2 & \cdots & n \\ \sigma(1) & \sigma(2) & \cdots & \sigma(n) \end{pmatrix}$$

The second standard notation for a permutation is known as cycle notation. It is more compact and will thus be used. A **k-cycle** is a sequence $(j_1 j_2 \dots j_k)$ of elements from $\{1, 2, \dots, n\}$ that denotes the permutation for which $\sigma(j_1) = j_2$, $\sigma(j_2) = j_3$, ..., $\sigma(j_{k-1}) = j_k$, $\sigma(j_k) = j_1$.

Example 2.6. Consider the permutation σ in the symmetric group S_4 such that $\sigma(1) = 4$, $\sigma(2) = 1$, $\sigma(3) = 3$, and $\sigma(4) = 2$.

In Cauchy notation:

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 4 & 1 & 3 & 2 \end{pmatrix}$$

In cycle notation:

$$\sigma = (142)(3) = (142)$$

¹ This notation is attributed to Augustin-Louis Cauchy [10]

1-cycles are often left out, but sometimes showing them is useful². Also, the starting element may vary, so the cycles (142) and (421) are equivalent.

Theorem 2.7. *Let $\sigma \in S_n$. There exists a unique product of disjoint k -cycles $\tau_1, \tau_2, \dots, \tau_m$ (including 1-cycles) such that $\sigma = \tau_1\tau_2\dots\tau_m$. \square*

The product in Theorem 2.7 is unique up to the order of the k -cycles, and is known as the **complete factorization** of the permutation σ .

Definition 2.8. *Let G be a group and let X be a set. A map $\gamma : G \times X \rightarrow X$ defined by $\gamma(g, x) = gx$ is said to be a **left group action** if the following conditions hold:*

- (i) $ex = x$, when e is the identity element of G .
- (ii) $(gh)(x) = g(h(x))$ for all $g, h \in G$.

One says that G **acts** on X . When G is a permutation group, the action that sends $(g, x) \rightarrow gx$ is known as the **natural action**. It will be assumed unless otherwise stated.

Definition 2.9. *Let the group G act on the set X . If $x \in X$, then the **orbit** of x is the set*

$$Gx = \{gx \mid g \in G\}.$$

Let $A \subset X$. The **stabilizer** of A is the subgroup of G defined by

$$G_A = \{g \in G \mid ga \in A \text{ for all } a \in A\}.$$

If $A = \{x\}$ is a singleton set, then the stabilizer of $\{x\}$ is $G_x = \{g \in G \mid gx = x\}$. When a group G acts on a set X , a permutation $g \in G$ may keep an element $x \in X$ **fixed**, i.e. $gx = x$. The set of all such fixed points of g is denoted by $\text{Fix}(g) = \{x \in X \mid gx = x\}$

Lemma 2.10. *If the group G acts on the non-empty set X , then the set of all orbits, denoted by X/G , forms a partition of X .*

Proof. Let $A \in X/G$. The orbit A is clearly non-empty since $A = Gx$ for some $x \in X$ and $Gx \neq \emptyset$ for all $x \in X$. Since $ex = x$ for all $x \in X$, each x belongs to some orbit in X/G . Hence $\cup_{A \in X/G} A = X$. Now it remains to be shown that the union of any two orbits are disjoint. Suppose not, then there exists $x \in X$ such that $x \in A$ and $x \in B$ but $A \neq B$. Since $A = Gy$ and $B = Gz$ for some $y, z \in X$, we have $x = gy$ and $x = g'z$ for some $g, g' \in G$. Now since $A \neq B$, and we can assume WLOG $A \supsetneq B$, i.e. there exists $a \in Gy$ such that $a \notin Gz$. Because $a = hy$ for some $h \in G$ and $x = gy$, we have $h^{-1}a = g^{-1}x$. It follows that $a = hg^{-1}x = hg^{-1}g'z \in Gz$, which is a contradiction. Therefore the union of any two orbits is disjoint. Thus all conditions of a partition are satisfied. \square

² For example in section 4.1.

Example 2.11. Here are some examples.

- 1 Let $G = (\mathbb{Q} \setminus 0, \cdot)$, and $X = \mathbb{R}$. Now G acts on \mathbb{R} as regular (left) multiplication. The orbits of each $x \in \mathbb{R}$ is the set $Gx = \{qx \mid q \in \mathbb{Q}\}$ and the stabilizer of each x is the multiplicative identity 1. The stabilizer of the set $A = \{\frac{\pi}{2^n} \mid n \in \mathbb{Z}\} \subseteq \mathbb{R}$ is the subgroup $G_A = \{\frac{1}{2^n} \mid n \in \mathbb{Z}\} \leq G$.
- 2 Let $G = \{e, (135)(246), (531)(642), (15)(24), (26)(35), (46)(13)\} \leq S_6$ and X the set of corners of the hexagon $\{1, 2, 3, 4, 5, 6\}$. Now G acts on X by permuting the corners. The orbit $G3 = \{1, 3, 5\}$, the stabilizer $G_3 = e$ and $X/G = \{\{1, 3, 5\}, \{2, 4, 6\}\}$.

Theorem 2.12. (The Orbit-stabilizer theorem) If the group G acts on a set X and $x \in X$, then there exists a bijection $f : G/G_x \rightarrow Gx$ such that $f(gG_x) = gx$.

Proof. First we show that the function $f : G/G_x \rightarrow Gx$, is well defined when $f(gG_x) = gx$. Let g and g' belong to the same coset in G/G_x . Now $g = g'h$ for some $h \in G_x$. Since $h \in G_x$ it holds that $gx = (g'h)x = g'(hx) = g'x$. Now we show that f is injective. Let $g'x = gx$. Now $g^{-1}g'x = x$, so $g^{-1}g' \in G_x$, which implies $g' \in gG_x$. Since also $g \in gG_x$, we have g and g' belonging to the same coset, and thus f is injective. Since f is clearly surjective, the proof is complete. \square

It has been shown that the number of left cosets of G_x is equal to the number elements in the orbit Gx , i.e. $[G : G_x] = |Gx|$. Thus, together with Lagrange's theorem (2.4), the orbit-stabilizer theorem states that $|G| = |G_x||Gx|$.

Definition 2.13. The **cyclic group** C_n is the group of rotational symmetries of the regular n -gon. The **dihedral group** D_n is the group of rotational and reflective symmetries of a regular n -gon. The **alternating group** A_n is a subgroup of S_n with index equal to 2.

An n -gon has n symmetric rotations and n symmetric reflections, hence the order of C_n is n and D_n is $2n$. Since $|S_n| = n!$, we have $|A_n| = \frac{n!}{2}$.

Example 2.14. Let $n = 5$. Now D_5 is the group of symmetries of the regular pentagon. These include the possible rotations and reflections. All 10 possible symmetries of the pentagon are listed in Figure 2.1 below.

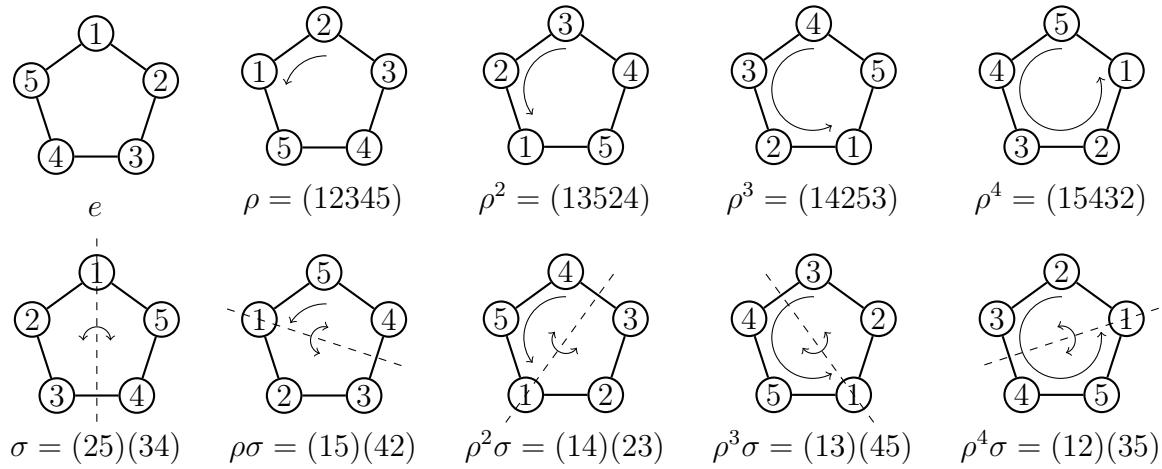


Fig. 2.1: Symmetries of a Regular Pentagon

2.2 Equivalence Relations

Definition 2.15. A binary relation \sim on a set X is said to be an **equivalence relation** if the following properties hold for all elements a , b , and c in X :

- (i) $a \sim a$. (Reflexivity)
- (ii) If $a \sim b$, then $b \sim a$. (Symmetry)
- (iii) If $a \sim b$ and $b \sim c$, then $a \sim c$. (Transitivity)

Two elements a , $b \in X$ are said to be **equivalent** if $a \sim b$. The **equivalence class** of an element $a \in X$, denoted by $[a]$, is the set $\{x \in X \mid x \sim a\}$.

Example 2.16. Let $p \in \mathbb{Z}$ be prime. Suppose for all a , $b \in \mathbb{Z}$ it holds that $a \sim b \Leftrightarrow a \equiv b \pmod{p}$. Now \sim is an equivalence relation because modular arithmetic is reflexive, symmetric, and transitive. An equivalence class $[a] \subset \mathbb{Z}$ is the set of all integers which equal $a \pmod{p}$. All the equivalence classes of \mathbb{Z} are thus $[0]$, $[1]$, $[2]$, ..., $[p-1]$.

Example 2.17. From lemma 2.10 we saw that the set of orbits X/G always partitions X . Now each of the orbits $A \in X/G$ induces a natural equivalence class X/\sim , where $a \sim b$ if and only if $a = gb$ for some $g \in G$. Reflexivity holds since $a = ea$, where e is the identity element of G . Symmetry holds since $a = gb \Rightarrow g^{-1}a = b$. Transitivity holds since if $a = gb$ and $b = g'c$ then $a = gg'c$.

Example 2.18. Suppose X and Y are finite sets, G is a group acting on the set X . An equivalence relation \sim on Y^X , the set of all functions from X to Y , can be defined as follows:

$$f_1 \sim f_2 \iff \exists g \in G \text{ such that } f_1(gx) = f_2(x) \text{ for all } x \in X.$$

The verification that \sim is an equivalence relation is straightforward. Choosing $g \in G$ to be the identity permutation we have $f_1(g(x)) = f_1(x)$ for all $x \in X$, thus $f_1 \sim f_1$ and reflexivity holds. If $f_1 \sim f_2$, then $f_1(g(x)) = f_2(x)$ for all $x \in X$. Now since $g^{-1} \in G$ and $f_1(x) = f_1(g^{-1}g(x)) = f_2(g^{-1}(x))$ for all $x \in X$, we have $f_2 \sim f_1$. Thus symmetry holds. If $f_1 \sim f_2$ and $f_2 \sim f_3$, then $\exists g_1, g_2 \in G$ such that $f_1(g_1(x)) = f_2(x)$ and $f_2(g_2(x)) = f_3(x)$ for all $x \in X$. Now since $g_1g_2 \in G$ and $f_1(g_1g_2(x)) = f_2(g_2(x)) = f_3(x)$, we have $f_1 \sim f_3$. Thus transitivity holds and hence \sim is an equivalence relation.

2.3 Generating Functions

The theory of generating functions in itself has rich applications to the theory of counting [9]. However, here only the basic idea is reviewed, as deeper parts of the theory are not needed to understand PET.

Definition 2.19. Let $a_0, a_1, a_2, a_3, \dots$ be a sequence of integers. The formal power series

$$G(a_n; x) = \sum_{n=0}^{\infty} a_n x^n = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \dots$$

is called the **generating function** associated with the sequence $a_0, a_1, a_2, a_3, \dots$. A generating function may have more than one variable, in which case it is known as a **multivariate generating function** and is of the form:

$$G(a_{(n_1, n_2, \dots, n_k)}; x_1, x_2, \dots, x_k) = \sum_{n_1, n_2, \dots, n_k=0}^{\infty} a_{n_1, n_2, \dots, n_k} x_1^{n_1} x_2^{n_2} \cdots x_k^{n_k}$$

Example 2.20. The following are some basic examples.

1. The generating function of the triangular numbers $1, 3, 6, 10, \dots$ is the power series

$$1 + 3x + 6x^2 + 10x^3 + \dots = \sum_{n=0}^{\infty} \binom{n+2}{2} x^n = \frac{1}{(1-x)^3}$$

2. The multivariate generating function for the binomial coefficients is

$$G(\binom{n}{k}; x, y) = \sum_{n=0}^{\infty} \binom{n}{k} x^k y^n = \frac{1}{1-y-xy}$$

3 Burnside's Lemma

PET relies heavily on a result from group theory which is often known as Burnside's lemma. Therefore, discussing it is necessary before tackling PET. Burnside's lemma gets its name after William Burnside, although it was known to Frobenius and in its essence to Cauchy. It is thus sometimes also called the Cauchy-Frobenius Lemma.[7] Another name for Burnside's lemma, which sheds more light on its function, is the orbit-counting theorem.

3.1 Burnside's Lemma

Theorem 3.1. (Burnside's Lemma) *Let a finite group G act on the set X . The total number of orbits, denoted by $|X/G|$, is given by*

$$|X/G| = \frac{1}{|G|} \sum_{g \in G} |Fix(g)|.$$

Burnside's lemma essentially states that the number of orbits is equal to the average number of elements in X which are fixed by each $g \in G$.

Proof. First we notice that $g \in G_x$ if and only if $x \in Fix(g)$. Thus we have

$$\sum_{x \in X} |G_x| = |\{(g, x) \in G \times X \mid gx = x\}| = \sum_{g \in G} |Fix(g)| \quad (3.1)$$

From the orbit-stabilizer theorem 2.12 we have that $[G : G_x] = |Gx|$, and together with Lagrange's theorem, $|G|/|G_x| = |Gx|$. Thus $|G|/|Gx| = |G_x|$, which substituted into the equation 3.1 above gives

$$\sum_{x \in X} \frac{|G|}{|Gx|} = |G| \sum_{x \in X} \frac{1}{|Gx|} = \sum_{g \in G} |Fix(g)| \quad (3.2)$$

By Lemma 2.10 we know that the set of orbits partitions the set X . Thus unions of orbits are disjoint and we can write

$$\sum_{x \in X} \frac{1}{|Gx|} = \sum_{A \in X/G} \sum_{x \in A} \frac{1}{|A|} = \sum_{A \in X/G} 1 = |X/G| \quad (3.3)$$

Combining equations 3.2 and 3.3 gives

$$|X/G| = \frac{1}{|G|} \sum_{g \in G} |Fix(g)|$$

□

3.2 Coloring the Cube

To demonstrate Burnside's lemma for counting colorings of an object with symmetries, we take a look at the following example.

Example 3.2. Let G be the group of rotational symmetries of the cube in three dimensions. Using Burnside's lemma, we derive a formula for the number of essentially different ways to color the faces of the cube with n given colors. Two colorings are considered equivalent if they differ only by a rotation of the cube. The axes of rotational symmetries of a cube are given in Figure 3.1 below.

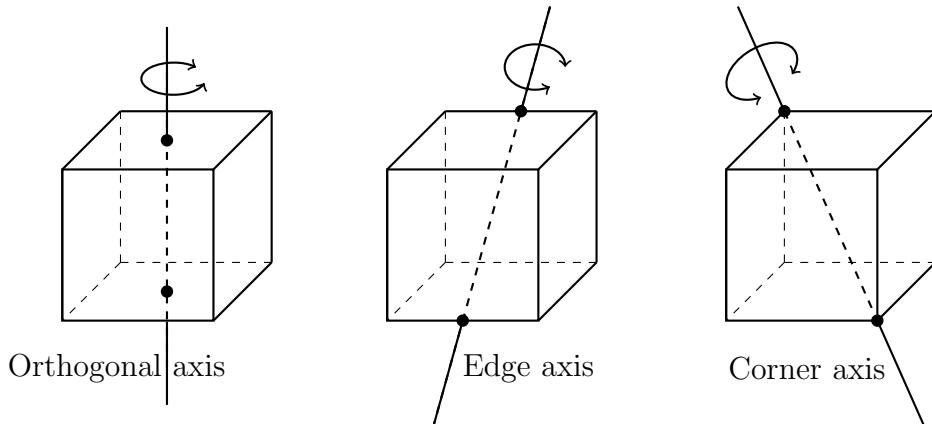


Fig. 3.1: The axes of symmetry for a cube

There are 4 possible rotations around an orthogonal axis (0, 90, 180, and 360 degrees), 2 rotations around an edge axis (0 and 180 degrees), and 3 rotations around a corner axis (0, 120 and 240 degrees). Since G is generated by these distinct rotations, $|G| = 4 \cdot 2 \cdot 3 = 24$. We proceed by numbering the faces of the cube 1, 2, 3, 4, 5, 6 as shown in Figure 3.2.

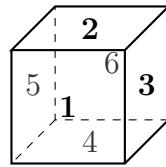


Fig. 3.2: Numbering of the cube's faces

Since colorings are equivalent if they differ only by a rotation, they are equivalent if they belong to the same orbit of G when G acts on the set of faces of the cube. Thus finding distinct colorings reduces to finding the number of orbits of G , and hence Burnside's lemma can be applied. We need to first find the number of fixed points for each $g \in G$. If g is the identity rotation, the number of different coloring of the cube is simply n^6 . If $g = (1)(6)(2345)$, it is a 90° rotation around the orthogonal axis. Since g holds faces 1 and 6 fixed, and each can be colored with n colors, there are n^2 distinct colorings for them. The remaining faces 2, 3, 4, and 5 are not fixed, but they are in the same cycle, so they must all be the same color to be invariant under g . Thus they can be colored in n possible ways. The total number of colorings under g is now $n^2n = n^3$. In a similar manner the number of fixed colorings of all 24 permutations in G can be found. One may notice that the number of fixed colorings is the number of cycles in g , including the unit cycles. This is no coincidence, and will be discussed in detail in section 4.1. Table 3.1 shows all 24 permutations in G and the number of colorings which they keep fixed.

Axis and degrees of rotation	Face permutations $g \in G$	$ Fix(g) $
Identity rotation	$(1)(2)(3)(4)(5)(6)$	n^6
Orthogonal (90° and 270°)	$(1)(6)(2345)$ $(2)(4)(1563)$ $(3)(5)(1264)$ $(1)(6)(5432)$ $(2)(4)(3651)$ $(3)(5)(4621)$	n^3
Orthogonal (180°)	$(1)(6)(24)(35)$ $(2)(4)(16)(35)$ $(3)(5)(24)(16)$	n^4
Edge (180°)	$(14)(26)(35)$ $(12)(46)(35)$ $(16)(45)(23)$ $(16)(34)(25)$ $(24)(13)(56)$ $(24)(15)(36)$	n^3
Corner (120° and 240°)	$(154)(263)$ $(123)(456)$ $(152)(346)$ $(143)(256)$ $(451)(362)$ $(321)(654)$ $(251)(643)$ $(341)(652)$	n^2

Tab. 3.1: The number of fixed n -colorings for each permutation of the cube's faces.

Now by applying Burnside's lemma we get the total number of distinct colorings with n colors to be

$$\frac{1}{|G|} \sum_{g \in G} |Fix(g)| = \frac{1}{24}(n^6 + 6n^3 + 3n^4 + 6n^3 + 8n^2) \quad (3.4)$$

The first few values of $f(n) = \frac{1}{24}(n^6 + 6n^3 + 3n^4 + 6n^3 + 8n^2)$ are given below:

n	$f(n)$	n	$f(n)$
1	1	6	2226
2	10	7	5390
3	57	8	11712
4	240	9	23355
5	800	10	43450

Tab. 3.2: The number of n -colorings of the cube under rotations.

4 The Cycle Index

We saw in chapter 3 the power of Burnside's lemma in its ability to take into account symmetries in counting. Using it, a formula for the n -colorings of the faces of a cube was found. Suppose, however, that we wish to find a formula for the n -colorings of the 32 sides of a truncated icosahedron. The problem could be solved by Burnside's lemma in exactly the same fashion as was done with the cube, but it would be extremely tedious, and therefore we seek a shortcut. This is where the cycle index comes to the rescue.

4.1 The Cycle Index

As mentioned in section 2.1, a permutation σ on a finite set X with n elements can be represented uniquely in its complete factorization $\sigma = \tau_1 \tau_2 \dots \tau_m$, where $m \leq n$. We say that σ is of **type** $\{b_1, b_2, \dots, b_n\}$ where b_i is the number i -cycles in the complete factorization $\tau_1 \tau_2 \dots \tau_m$. For example, the permutation $(1532)(46)(87)(9)$ is of type $\{1, 2, 0, 1, 0, 0, 0, 0, 0\}$.

Definition 4.1. *Let G be a group of permutations. The **cycle index** is the polynomial with n variables x_1, x_2, \dots, x_n*

$$Z_G(x_1, x_2, \dots, x_n) = \frac{1}{|G|} \sum_{g \in G} x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n}$$

where the product $x_1^{b_1} x_2^{b_2} \cdots x_n^{b_n}$ is formed for each $g \in G$ from its type $\{b_1, b_2, \dots, b_n\}$.¹

The cycle index depends on the structure of the group action G on the set X . Thus for each structure of G and different sizes of X we must find a new cycle index. For this reason finding the cycle index must be done in a case by case basis, as is done in the following examples from [2].

Example 4.2. *First we revisit the situation in Example 3.2, where we have that G is the group of rotational symmetries of the cube, and it acts on the faces of the cube. The*

¹ Pólya used the letter Z to hint at the German for cycle index, which is *zyklenzeiger*.[7]

identity rotation is written in cyclic form $(1)(2)(3)(4)(5)(6)$, so its type is $\{6, 0, \dots, 0\}$. Thus it contributes the monomial $x_1^{b_1}x_2^{b_2} \cdots x_n^{b_n} = x_1^6$ to the cycle index. The orthogonal rotation of 180° characterized by the permutation $(1)(6)(24)(35)$ is of type $\{2, 2, 0, \dots, 0\}$ so it contributes the monomial $x_1^2x_2^2$ to the cycle index. Continuing in this way through all $g \in G$, we get the cycle index

$$Z_G(x_1, x_2, x_3, x_4) = \frac{1}{24}(x_1^6 + 6x_1^2x_4 + 3x_1^2x_2^2 + 6x_2^3 + 8x_3^2). \quad (4.1)$$

Substituting $x_i = n$ for all i in equation 4.1 gives equation 3.4.

Example 4.3. Suppose G is again the group of rotational symmetries of the cube, but this time it acts on the set of vertices of the cube V , where $|V| = 8$. We have the same sets of rotational symmetries:

- (a) Identity rotation.
- (b) Six rotations of the orthogonal axis by 90° and 270° .
- (c) Three rotations of the orthogonal axis by 180° .
- (d) Six rotations of the edge axis by 180° .
- (e) Eight rotations of the corner axis by 120° and 240° .

In each case we can visualize the cycles, and directly pick out the cycle types. The identity rotation has type $\{8, 0, 0, \dots, 0\}$. The rotations in (b) have type $\{0, 0, 0, 2, 0, \dots, 0\}$. The rotations in (c) have type $\{0, 4, 0, 0, \dots, 0\}$. The rotations in (d) have type $\{0, 4, 0, \dots, 0\}$. The rotations in (e) have type $\{2, 0, 2, 0, \dots, 0\}$. Thus the cycle index is

$$Z_G(x_1, x_2, x_3, x_4) = \frac{1}{24}(x_1^8 + 6x_4^2 + 3x_2^4 + 6x_2^4 + 8x_1^2x_3^2).$$

Similarly, if G acts on the set of edges of the cube E , we can find the cycle index as follows, noting that $|E| = 12$. The identity rotation has type $\{12, 0, 0, \dots, 0\}$. The rotations in (b) have type $\{0, 0, 0, 3, 0, \dots, 0\}$. The rotations in (c) have type $\{0, 6, 0, 0, \dots, 0\}$. The rotations in (d) have type $\{2, 5, 0, \dots, 0\}$. The rotations in (e) have type $\{0, 0, 4, 0, \dots, 0\}$. Thus the cycle index is

$$Z_G(x_1, x_2, x_3, x_4) = \frac{1}{24}(x_1^{12} + 6x_4^4 + 3x_2^6 + 6x_1^2x_2^5 + 8x_3^4).$$

4.2 Special Cases

In his original 1937 paper, Pólya lists the cycle indices of some special cases. In particular, he gives them for the natural actions of common subgroups of the symmetric group.

The Trivial Permutation Group

The trivial permutation group $E_n \leq S_n$ is the permutation group containing only the identity permutation. The cycle index is

$$Z_{E_n}(x_1) = x_1^n$$

The Cyclic Group

The cyclic permutation group $C_n \leq S_n$ is the permutation group which contains all cyclic permutations of n elements. It can be thought of as the group of rotational symmetries of an n -gon. The cycle index is then given by

$$Z_{C_n}(x_1, x_2, \dots, x_n) = \frac{1}{n} \sum_{d|n} \phi(d) x_d^{n/d}$$

where ϕ is the Euler totient function.[7]

Example 4.4. *In the case $n = 5$, C_5 is the group of rotational symmetries of the pentagon. The cycle index is then*

$$\begin{aligned} Z_{C_5}(x_1, x_2, \dots, x_n) &= \frac{1}{5} \sum_{d|5} \phi(d) x_d^{5/d} \\ &= \frac{1}{5} (x_1^5 + 4x_5). \end{aligned}$$

The Dihedral Group

The dihedral group D_n , as in definition 2.13, includes the rotations and reflections of the n -gon. The cycle index now varies depending of whether n is even or odd.[7]

$$Z_{D_n}(x_1, x_2, \dots, x_n) = \frac{1}{2} Z_{C_n}(x_1, x_2, \dots, x_n) + \begin{cases} \frac{1}{2} x_1 x_2^{(n-1)/2} & \text{if } n \text{ is odd} \\ \frac{1}{4} (x_1^2 x_2^{(n-2)/2} + x_2^{n/2}) & \text{if } n \text{ is even} \end{cases}$$

The Symmetric Group²

Let (j) denote a partition of n , that is, $(j) \in \{(j_1, j_2, \dots, j_n) \mid j_1 + 2j_2 + \dots + nj_n = n\}$.

² In [7] Pólya gives only the cycle index for cases $n = 1, 2, 3, 4$ for the symmetric group and alternating group. The general cases are given by Harary and Palmer in [4].

The cycle index of the symmetric group acting on a set of n elements is then given by:

$$Z_{S_n}(x_1, x_2, \dots, x_n) = \sum_{(j)} \frac{1}{\prod k^{j_k} j_k!} \prod_{k=1}^n x_k^{j_k}$$

where the sum is taken over all partitions of n .

The Alternating Group

The cycle index of the alternating group acting on a set of n elements is given by

$$Z_{A_n}(x_1, x_2, \dots, x_n) = Z_{S_n}(x_1, x_2, \dots, x_n) + Z_{S_n}(x_1, -x_2, x_3, -x_4, \dots, \pm x_n).$$

5 Pólya's Enumeration Theorem

5.1 Configurations and Weights

In this section we define the concept of a “configuration” along with its “weight” in the context of Pólya theory. Throughout the section we will focus on functions between two finite sets, X and Y . The set of all function from X to Y is denoted by Y^X , and it is well known that its cardinality is given by $|Y|^{|X|}$.

Definition 5.1. Let X and Y be finite sets, with the group G acting on the set X . Let \sim be the equivalence relation on Y^X given by

$$f_1 \sim f_2 \iff \exists g \in G \text{ such that } f_1(gx) = f_2(x) \text{ for all } x \in X.$$

The equivalence classes of \sim will be called **configurations**.²

Example 5.2. Let $X = \{1, 2, 3, 4, 5\}$ be the set of numbered edges of a pentagon, let G be the cyclic group C_5 , and Y the set containing the words “black” and “white”.

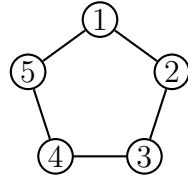


Fig. 5.1: Pentagon with numbered corners.

There are now eight distinct configurations, as seen in Figure 5.2

¹ The verification that \sim is an equivalence relation was done in example 2.18.

² Some authors, such as De Bruijn and Graver, call these equivalence classes “patterns”.

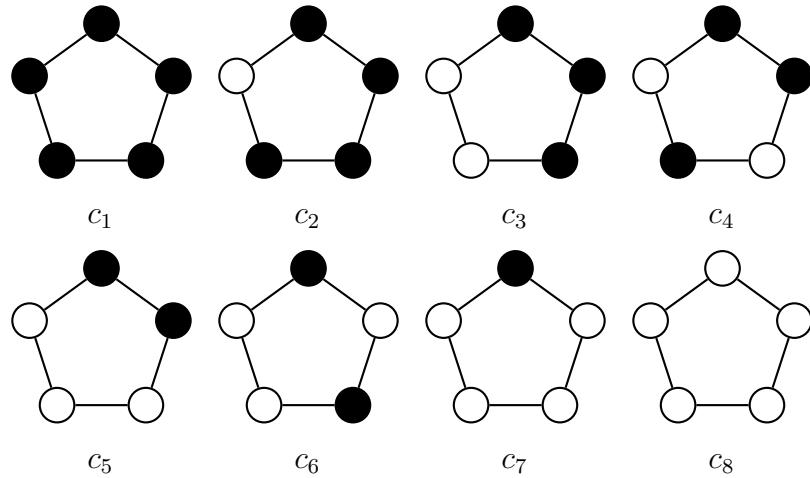


Fig. 5.2: The 8 distinct 2-colorings of the corners of a pentagon under rotational symmetry.

The eight configurations can be represented by the symbols c_1, c_2, \dots, c_8 . For example, c_5 represents the configuration in which two adjacent corners are black and the rest are white. Let us define functions f_1 and f_2 as follows:

$$f_1(x) = \begin{cases} \text{black, if } x \in \{1, 2\} \\ \text{white, if } x \in \{3, 4, 5\} \end{cases} \quad f_2(x) = \begin{cases} \text{black, if } x \in \{3, 4\} \\ \text{white, if } x \in \{1, 2, 5\} \end{cases}$$

Now both f_1 and f_2 belong to the configuration c_5 , because letting $g = (14253)$ we have $f_1(g(x)) = f_2(x)$ for all $x \in X$.

The next lemma shows how the number of configurations is related to the group G .

Lemma 5.3. If C denotes the set of configurations of Y^X , and G is a permutation group acting on X , then the number of configurations of Y^X is given by

$$|C| = \frac{1}{|G|} \sum_{g \in G} |\{f : X \rightarrow Y \mid f = fg\}|.$$

Proof. We begin by using the group G acting on X to define a group G' acting on Y^X . Consider the set $\{\pi_g : Y^X \rightarrow Y^X \mid \pi_g(f) = fg^{-1}, g \in G\}$ with the composition of functions operation. We show that this is a group acting on Y^X , denoting it by G' .

First we note that for all $g, h \in G$ we have $\pi_g \pi_h(f) = fh^{-1}g^{-1} = f(gh)^{-1} = \pi_{gh}(f)$. Closure under the composition of functions operation then follows from $\pi_g \pi_h = \pi_{gh} \in G'$. Associativity also holds as $\pi_g(\pi_h \pi_j) = \pi_g \pi_{hj} = \pi_{ghj} = \pi_{gh} \pi_j = (\pi_g \pi_h) \pi_j$. The identity element of G' is π_e , where e is the identity element of G , since $\pi_e \pi_g = \pi_{eg} = \pi_g$.

for all $\pi_g \in G'$. The inverse element of π_g is $\pi_{g^{-1}}$ since $\pi_g \pi_{g^{-1}} = \pi_{g g^{-1}} = \pi_e$. Thus G' is a group of permutations on Y^X and it acts on Y^X because $\pi_e(f) = f e = f$ and $(\pi_g \pi_h)(f) = \pi_{gh}(f) = f(gh)^{-1} = f h^{-1} g^{-1} = \pi_g(\pi_h(f))$. Let \mathcal{O} denote an orbit in Y^X/G' and let D denote a configuration in C . Now

$$\begin{aligned} f_1, f_2 \in \mathcal{O} &\Leftrightarrow f_1 = \pi_g(f_2) = f_2 g^{-1} \text{ for some } g \in G \\ &\Leftrightarrow f_1 g = f_2 \text{ for some } g \in G \\ &\Leftrightarrow f_1, f_2 \in D. \end{aligned}$$

Hence functions belong to the same orbit of Y^X/G' iff they belong to the same configuration in C , and therefore

$$|C| = |Y^X/G'|. \quad (5.1)$$

Applying Burnside's lemma (theorem 3.1) to the RHS of equation 5.1 gives:

$$|C| = \frac{1}{|G'|} \sum_{\pi_g \in G'} |\text{Fix}(\pi_g)|. \quad (5.2)$$

Next we note that since $\pi_g(f) = f \Leftrightarrow f = f g^{-1} \Leftrightarrow f = f g$, we have

$$\text{Fix}(\pi_g) = \{f : X \rightarrow Y \mid \pi_g(f) = f\} = \{f : X \rightarrow Y \mid f = f g\}. \quad (5.3)$$

Finally substituting Equation 5.3 into Equation 5.2 and noting that $\pi_g \in G$ iff $g \in G$ gives the result

$$|C| = \frac{1}{|G|} \sum_{g \in G} |\{f : X \rightarrow Y \mid f = f g\}|.$$

□

In Example 5.2 the colors were represented by the words “black” and “white”, and configurations were represented with symbols c_1, c_2, \dots, c_8 . By introducing the concept of weights to the colors and configurations, we can manipulate them algebraically.

Definition 5.4. Let Y be a finite set, let R be a commutative ring which contains the rational numbers as a subset³, and let $w : Y \rightarrow R$. The **weight** of each $y \in Y$ is the element $w(y)$. The **weight of a function** $f : X \rightarrow Y$, denoted by $W(f)$, is the product:

$$W(f) = \prod_{x \in X} w(f(x)).$$

³ For example a polynomial ring $\mathbb{Q}[X_1, \dots, X_n]$. This construction allows for the multiplication of weights by rational coefficients in the cycle index.

The weight function w allow elements in Y to borrow the algebraic structure of R , so that they can be manipulated indirectly with $w \circ f$. The following diagram illustrates the situation:

$$\begin{array}{ccc} X & \xrightarrow{w \circ f} & R \\ & \searrow f & \uparrow w \\ & Y & \end{array}$$

Fig. 5.3: The weight function w .

The weights of all functions belonging to the same configuration are equivalent, as seen in the following lemma:

Lemma 5.5. *Let $D \subseteq Y^X$ be a configuration. If two functions $f_1, f_2 \in D$ then*

$$W(f_1) = W(f_2).$$

Proof. Let $f_1, f_2 \in D$. By definition there exists $g \in G$ such that $f_1(gx) = f_2(x)$. Now

$$W(f_1) = \prod_{x \in X} w(f_1(x)) = \prod_{x \in X} w(f_1(gx)) = \prod_{x \in X} w(f_2(x)) = W(f_2).$$

□

Definition 5.6. *The **weight of a configuration** is defined to be the common weight of all functions in the configuration. If D is a configuration, the weight of D is denoted by $W(D)$.*

Example 5.7. *Continuing with example 5.2, we can assign weights $w(\text{black}) = B$, and $w(\text{white}) = W$, where B and W are elements of the polynomial ring $\mathbb{Q}[B, W]$. Now the functions f_1 and f_2 have the same weight*

$$\begin{aligned} W(f_1) &= \prod_{x \in X} w(f_1(x)) \\ &= w(f_1(1))w(f_1(2))w(f_1(3))w(f_1(4))w(f_1(5)) \\ &= BBWWWW \\ &= B^2W^3 \end{aligned}$$

Thus the weight of c_5 is $W(c_5) = W(f_1) = B^2W^3$.

Next we prove a lemma which will be useful for proving Pólya's enumeration theorem.

Lemma 5.8. *Let X be a disjoint union of sets X_1, X_2, \dots, X_n . If $S \subset Y^X$ is the set of functions f which are constant on each X_i , then*

$$\sum_{f \in S} W(f) = \prod_{i=1}^n \sum_{y \in Y} w(y)^{|X_i|}$$

Proof. Suppose $Y = \{y_1, \dots, y_m\}$. We begin by expanding the product

$$\prod_{i=1}^k \sum_{y \in Y} w(y)^{|X_i|} = (w(y_1)^{|X_1|} + \dots + w(y_m)^{|X_1|}) (w(y_1)^{|X_2|} + \dots + w(y_m)^{|X_2|}) \dots (w(y_1)^{|X_n|} + \dots + w(y_m)^{|X_n|}). \quad (5.4)$$

Multiplying out the RHS of equation 5.4 gives a sum

$$(w(y_1)^{|X_1|} w(y_1)^{|X_2|} \dots w(y_1)^{|X_n|}) + (w(y_1)^{|X_1|} w(y_1)^{|X_2|} \dots w(y_2)^{|X_n|}) + \dots + (w(y_m)^{|X_1|} w(y_m)^{|X_2|} \dots w(y_m)^{|X_n|}). \quad (5.5)$$

Since f is constant in each X_i iff $f \in S$, each term in this sum corresponds to a single function $f \in S$. Thus the sum 5.5 can be written as

$$\sum_{f \in S} w(f(x_1))^{|X_1|} w(f(x_2))^{|X_2|} \dots w(f(x_n))^{|X_n|} \quad (5.6)$$

where $x_i \in X_i$ for each $i \in \{1, \dots, n\}$. Finally we notice that 5.6 can also be written as

$$\begin{aligned} & \sum_{f \in S} \left(\prod_{x \in X_1} w(f(x)) \right) \left(\prod_{x \in X_2} w(f(x)) \right) \dots \left(\prod_{x \in X_n} w(f(x)) \right) \\ &= \sum_{f \in S} \prod_{x \in X} w(f(x)) \\ &= \sum_{f \in S} W(f) \end{aligned}$$

Thus the lemma holds. \square

5.2 The Configuration Generating Function

Given a set of configurations C on Y^X , the **configuration generating function** (or CGF) is defined by

$$F(C) = \sum_{c \in C} W(c).$$

Example 5.9. Given the situation in example 5.2, the set of configurations is $C = \{c_1, c_2, \dots, c_8\}$. Thus the CGF becomes

$$\begin{aligned}\sum_{c \in C} W(c) &= W(c_1) + W(c_2) + \dots + W(c_8) \\ &= B^5 + B^4W + B^3W^2 + B^3W^2 + B^2W^3 + B^2W^3 + BW^4 + W^5 \\ &= B^5 + B^4W + 2B^3W^2 + 2B^2W^3 + BW^4 + W^5.\end{aligned}$$

The CGF thereby lists all possible weights of configurations with the coefficient representing the number configurations with the given weight. For example, the weight B^2W^3 has coefficient 2, so we know that there are two distinct configurations with weight B^2W^3 . In other words there are two distinct colorings of the corners of the pentagon such that two corners are black and three are white. Thus knowing the CGF, we know how many distinct colorings there are for each set of weights. To find the total number of colorings, we can simply assign weights $w(\text{white}) = w(\text{black}) = 1$ which gives $W(c_i) = 1$ for all i . Now the CGF gives $F(C) = 8$, the number of distinct colorings.

5.3 Pólya's Enumeration Theorem

Theorem 5.10. (Pólya's Enumeration Theorem) Let X and Y be finite sets, with $|X| = n$. Let G be a group acting on X and let Z_G be the cycle index polynomial. If w is the weight function on Y , then the configuration generating function is given by:

$$Z_G \left(\sum_{y \in Y} w(y), \sum_{y \in Y} w(y)^2, \dots, \sum_{y \in Y} w(y)^n \right).$$

The special case of assigning $w(y) = 1$ for all $y \in Y$ gives the total number of configurations: $Z_G(|Y|, |Y|, \dots, |Y|)$.

Proof. Let $S_\omega \subseteq Y^X$ be the set of functions that have weight ω . Let $\phi_\omega(g) = \{f : X \rightarrow Y \mid f = fg, W(f) = \omega\}$. By lemma 5.3 the number of configurations in S_ω is given by

$$|S_\omega| = \frac{1}{|G|} \sum_{g \in G} |\phi_\omega(g)|. \quad (5.7)$$

Thus multiplying by ω and summing over all values of ω gives the CGF:

$$\sum_{c \in C} W(c) = \sum_{\omega} \omega |S_\omega| = \frac{1}{|G|} \sum_{\omega} \sum_{g \in G} \omega |\phi_\omega(g)|. \quad (5.8)$$

Letting $\phi(g)$ denote the set $\{f : X \rightarrow Y \mid f = fg\}$, we have that

$$\sum_{\omega} \omega |\phi_\omega(g)| = \sum_{f \in \phi(g)} W(f). \quad (5.9)$$

Since the double summation in 5.8 is taken over finite sets, the order of the summation may be switched. Thus switching the order of summation and combining with 5.9 gives the CGF

$$\sum_{c \in C} W(c) = \frac{1}{|G|} \sum_{g \in G} \sum_{f \in \phi(g)} W(f). \quad (5.10)$$

Every $g \in G$ permutes the set X . Therefore each g splits X into a disjoint union of m cycles X_1, X_2, \dots, X_m , where $m \leq n$. If $f \in S$, then $f = fg = fg^2 = \dots$, i.e. f is constant on each X_i . If f is constant on each X_i , then $f = fg$, and hence $f \in S$. Now applying lemma 5.8 gives

$$\sum_{f \in \phi(g)} W(f) = \prod_{i=1}^m \sum_{y \in Y} w(y)^{|X_i|} = \left(\sum_{y \in Y} w(y)^{|X_1|} \right) \left(\sum_{y \in Y} w(y)^{|X_2|} \right) \dots \left(\sum_{y \in Y} w(y)^{|X_m|} \right). \quad (5.11)$$

If the cycle type of g is $\{b_1, b_2, \dots, b_n\}$, then in $|X_1|, |X_2|, \dots, |X_m|$, the number i occurs b_i times. Thus we can write 5.11 as

$$\sum_{f \in \phi(g)} W(f) = \left(\sum_{y \in Y} w(y) \right)^{b_1} \left(\sum_{y \in Y} w(y)^2 \right)^{b_2} \dots \left(\sum_{y \in Y} w(y)^n \right)^{b_n}. \quad (5.12)$$

Substituting equation 5.12 into 5.10 gives the CGF:

$$\frac{1}{|G|} \sum_{g \in G} \left(\left(\sum_{y \in Y} w(y) \right)^{b_1} \left(\sum_{y \in Y} w(y)^2 \right)^{b_2} \dots \left(\sum_{y \in Y} w(y)^n \right)^{b_n} \right). \quad (5.13)$$

Now we simply notice that 5.13 is precisely the cycle index

$$Z_G \left(\sum_{y \in Y} w(y), \sum_{y \in Y} w(y)^2, \dots, \sum_{y \in Y} w(y)^n \right).$$

This proves Pólya's Enumeration Theorem. □

6 Applications

The beauty in PET is its generality, which leads to a diverse set of applications. In his 1937 paper Pólya gave applications of PET in the enumeration of graphs and chemical compounds. Since then, as PET came to the attention of the wider mathematical community, numerous new applications have been found. Within mathematics, applications apart from graph theory include those in logic, number theory, and the study of quadratic forms. Applications outside of mathematics are found in physics, chemistry, and even music theory.[7]

This chapter begins by discussing the applications of PET to the coloring of polytopes of dimension 2 and 3. Then we take a look at how PET can, perhaps unexpectedly, be used in number theory to produce a neat generalization of Fermat's theorem and Gauss' theorem. In the theory of graphical enumeration, the important applications of PET in enumerating trees and (v, e) -graphs is discussed. The chapter is concluded with some of Pólya's examples in chemical enumeration.

6.1 Coloring Polytopes in Dimensions 2 and 3

In this section some natural applications of PET are given in the coloring of polygons and polyhedra. The theory is the same for higher dimensional polytopes, but visualization becomes difficult. Some examples given in this section are ones which have been partially discussed in earlier chapters. Particularly the coloring of the cube is presented again so that the reader may appreciate the simplicity and generality of PET in comparison to Burnside's lemma.

6.1.1 Necklaces

The regular polygons with colored vertices are sometimes called necklaces, and the vertices are called beads. PET can be used to enumerate the number of beaded necklaces with n colors.

Example 6.1. *Given a set of black and white beads, how many distinct five beaded necklaces can be made if one allows for rotation of the necklaces? How many of them contain two black beads and three white beads?*

We let X be a five beaded necklace, and Y be the set containing the two colors black and white. The relevant permutation group G is the cyclic group C_5 . We assign weights to the two colors as follows: $w(\text{black}) = B$ and $w(\text{white}) = W$. Now applying PET gives the CGF:¹

$$\begin{aligned} F(B, W) &= Z_G(B + W, B^2 + W^2, \dots, B^5 + W^5) \\ &= \frac{1}{5}((B + W)^5 + 4(B^5 + W^5)) \\ &= B^5 + B^4W + 2B^3W^2 + 2B^2W^3 + BW^4 + W^5 \end{aligned}$$

To find the number of distinct necklaces which contain two black beads and three white beads we simply read off from the CGF the coefficient of the term B^2W^3 , which is 2. To find the total number necklaces, we assign weights $w(\text{white}) = w(\text{black}) = 1$, which gives $F(1, 1) = 1 + 1 + 2 + 2 + 1 + 1 = 8$. This matches our earlier result in Example 5.7, and these 8 necklaces were shown in Figure 5.2.

Now a slightly more general necklace problem.

Example 6.2. Assume that two necklaces are identical if one can be formed from the other by rotations and/or reflections. We find the general formula for the number of necklaces that can be made with k_1 black beads and k_2 white beads, where $k_1 + k_2$ is an odd prime and $k_1, k_2 \neq 0$.²

First we let k_1 and k_2 be positive integers such that $k_1 + k_2 = n$, where n is an odd prime. Since n is odd, we can assume without loss of generality that k_1 is even. We assign weights B and W to the black and white beads respectively. Now the relevant group acting on the necklace is the dihedral group and since n is odd, we find the cycle index from section 4.2 to be:

$$Z_{D_n}(x_1, x_2, \dots, x_n) = \frac{1}{2}Z_{C_n}(x_1, x_2, \dots, x_n) + \frac{1}{2}x_1x_2^{(n-1)/2} \quad (6.1)$$

Substituting the cycle index Z_{C_n} into equation 6.1 gives:

$$\begin{aligned} Z_{D_n}(x_1, x_2, \dots, x_n) &= \frac{1}{2n} \sum_{d|n} \phi(d)x_d^{n/d} + \frac{1}{2}x_1x_2^{(n-1)/2} \\ &= \frac{1}{2n}(x_1^n + (n-1)x_n) + \frac{1}{2}x_1x_2^{(n-1)/2} \end{aligned} \quad (6.2)$$

Using the cycle index in equation 6.2, we now apply PET to get the configuration generating function:

$$F(B, W) = \frac{1}{2n}(B + W)^n + \frac{1}{2n}(n-1)(B^n + W^n) + \frac{1}{2}(B + W)(B^2 + W^2)^{(n-1)/2} \quad (6.3)$$

¹ All polynomial expansions in this section were done in Maple 2015.

² A similar problem was given as an exercise in [3].

We need not expand the polynomials since we are only interested in the coefficient of the term $B^{k_1}W^{k_2}$. We look separately at the three summands of equation 6.3. First we notice that the coefficient of $B^{k_1}W^{k_2}$ in $\frac{1}{2n}(B + W)^n$ is given by the binomial theorem as $\frac{1}{2n}\binom{n}{k_1}$. The second summand $\frac{1}{2n}(n-1)(B^n + W^n)$ does not affect the coefficient of $B^{k_1}W^{k_2}$, since it is only adding to the coefficients of B^n and W^n . In the final summand, using the binomial theorem we see that $(B^2 + W^2)^{(n-1)/2}$ contributes $\binom{(n-1)/2}{k_1/2}$ to the coefficient of $B^{k_1}W^{k_2-1}$. Then multiplying through by $\frac{1}{2}(B + W)$, the coefficient of $B^{k_1}W^{k_2}$ becomes $\frac{1}{2}\binom{(n-1)/2}{k_1/2}$. Having now accounted for each of the summands, the coefficient of the $B^{k_1}W^{k_2}$ term is given by the sum:

$$\frac{1}{2n}\binom{n}{k_1} + \frac{1}{2}\binom{(n-1)/2}{k_1/2} \quad (6.4)$$

Hence the general formula for the number of necklaces that can be formed using k_1 black beads and k_2 white beads, where $k_1 + k_2$ is an odd prime, is given by:

$$\frac{1}{2(k_1 + k_2)}\binom{k_1 + k_2}{k_1} + \frac{1}{2}\binom{(k_1 + k_2 - 1)/2}{k_1/2} \quad (6.5)$$

6.1.2 The Cube

Example 6.3. In how many ways can the six faces of a cube be colored such that three faces are red, two are blue, and one is purple?

Letting X be the set of six faces of the cube, and Y the set of colors with weights $w(\text{red}) = R$, $w(\text{blue}) = B$ and $w(\text{purple}) = P$. The appropriate permutation group is the group of rotational symmetries of the cube. The cycle index was found in Example 4.2 to be

$$Z_G(x_1, x_2, x_3, x_4) = \frac{1}{24}(x_1^6 + 6x_1^2x_4 + 3x_1^2x_2^2 + 6x_2^3 + 8x_3^2)$$

Now PET gives the CGF

$$\begin{aligned} F(R, B, P) &= Z_G((R + B + P), (R^2 + B^2 + P^2), \dots, (R^4 + B^4 + P^4)) \\ &= \frac{1}{24}((R + B + P)^6 + 6(R + B + P)^2(R^4 + B^4 + P^4) + \\ &\quad 3(R + B + P)^2(R^2 + B^2 + P^2)^2 + 6(R^2 + B^2 + P^2)^3 + \\ &\quad 8(R^3 + B^3 + P^3)^2) \\ &= R^6 + R^5B + R^5P + 2R^4B^2 + 2R^4BP + 2R^4P^2 + 2R^3B^3 + 3R^3B^2P + \\ &\quad 3R^3BP^2 + 2R^3P^3 + 2R^2B^4 + 3R^2B^3P + 6R^2B^2P^2 + 3R^2BP^3 + \\ &\quad 2R^2P^4 + RB^5 + 2RB^4P + 3RB^3P^2 + 3RB^2P^3 + 2RBP^4 + RP^5 + \\ &\quad B^6 + B^5P + 2B^4P^2 + 2B^3P^3 + 2B^2P^4 + BP^5 + P^6 \end{aligned}$$

The coefficient of R^3B^2P is 3, thus there are 3 distinct colorings of the cube such that three faces are red, two are blue and one is purple. The total number of 3-colorings of the cube is found by

$$Z_G(|Y|, |Y|, \dots, |Y|) = Z_G(3, 3, \dots, 3) = \frac{1}{24}(3^6 + 6 \cdot 3^23 + 3 \cdot 3^23^2 + 6 \cdot 3^3 + 8 \cdot 3^2) = 57$$

This matches the result in table 3.2 using Burnside's lemma.

6.1.3 The Truncated Icosahedron

Example 6.4. In how many different ways can the faces of a truncated icosahedron³ be colored such that 12 faces are black and 20 faces are white?

Let X be the set of 32 faces of the truncated icosahedron, and Y be the set containing the colors black and white. The appropriate group G is the group of rotational symmetries of the truncated icosahedron.

The first, and most tedious task, is finding the cycle index. A truncated icosahedron consists of 12 pentagons and 20 hexagons. The graphical representations in figure 6.1 help to visualize the truncated icosahedron. Each of the three graphs is centered at a different type of axis of rotational symmetry.

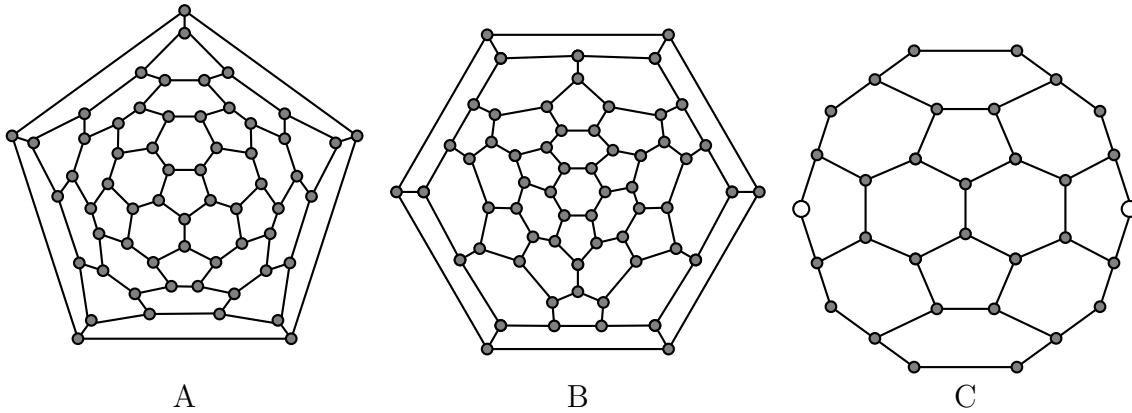


Fig. 6.1: The truncated icosahedron centered at the three different types of axes of rotational symmetry. A and B are Schlegel diagrams and C is an orthogonal projection.

To find the cycle index, we do not need to find all elements in G , it is sufficient to know their types. The type of the identity rotation is clearly $\{32, 0, \dots\}$. An axis of symmetry goes through the center of each pentagon, as shown in graph A of figure 6.1. Since there are 12 pentagons, and each pentagonal axis of symmetry goes through

³ Equivalently a classic soccer ball or buckminsterfullerene molecule.

two pentagons, there is a total of 6 such pentagonal axes of symmetry. Symmetries are formed by rotations of 72, 144, 216 and 288 degrees around such an axis. Thus there are $4 \cdot 6 = 24$ such pentagonal rotations in G . Under each rotation the center pentagon and outer pentagon remain fixed. Each other pentagon rotates to another pentagon which is the same distance from the center. The same holds for the hexagons. Thus such a rotation is of the form $(p_1) (p_2p_3p_4p_5p_6) (p_7p_8p_9p_{10}p_{11}) (p_{12}) (h_1h_2h_3h_4h_5) (h_6h_7h_8h_9h_{10}) (h_{11}h_{12}h_{13}h_{14}h_{15}) (h_{16}h_{17}h_{18}h_{19}h_{20})$. This rotation has type $\{2, 0, 0, 0, 6, 0, \dots\}$. Note that all symmetric rotations of the pentagon only permute the 5-cycles, they do not split them into smaller cycles. Now since we have a total of 24 rotations of pentagons, not including the identity rotation, they contribute the monomial $24x_1^2x_5^6$ to the cycle index.

Another axis of symmetry goes through the center of each hexagon. These can be visualized using the Schlegel diagram B in figure 6.1. There are a total of 10 such hexagonal axes of symmetry, where symmetries are formed by rotations of 120 and 240 degrees. Thus there are 20 rotations of hexagons in G . These rotations have the form $(p_1p_2p_3) (p_4p_5p_6) (p_7p_8p_9) (p_{10}p_{11}p_{12}) (h_1) (h_2h_3h_4) (h_5h_6h_7) (h_8h_9h_{10}) (h_{11}h_{12}h_{13}) (h_{14}h_{15}h_{16}) (h_{17}h_{18}h_{19}) (h_{20})$. Thus the cycle type for each such rotation is $\{2, 0, 10, 0, \dots\}$. Now since there are 20 rotations of hexagonal axes, they contribute the monomial $20x_1^2x_3^{10}$ to the cycle index.

The final axis of symmetry on the truncated icosahedron is the type that goes through the center of edges joining two hexagons. This is visualized by the orthogonal projection C in figure 6.1. There are 30 such edges, and since each axis of symmetry goes through two of them, there is a total of 15 of such edge axes. Each of them has 2-fold symmetry, hence there are 15 rotations around edge axes in G . The 180 degree rotation around an edge axis has the form $(p_1p_2) (p_3p_4) (p_5p_6) (p_7p_8) (p_9p_{10}) (p_{11}p_{12}) (h_1h_2) (h_3h_4) (h_5h_6) (h_7h_8) (h_9h_{10}) (h_{11}h_{12}) (h_{13}(h_{14})) (h_{15}h_{16}) (h_{17}h_{18}) (h_{19}h_{20})$. The cycle type of each such rotation is $\{0, 16, 0, \dots\}$. Since there are 15 such axes of symmetry, they contribute the monomial $15x_2^{16}$ to the cycle index.

Now including the identity rotation, we have found $1 + 24 + 20 + 15 = 60$ rotations. These are all possible rotations since the orbit-stabilizer theorem applied on a pentagonal face x gives $|G| = |G_x||Gx| = 5 \cdot 12 = 60$. The cycle index is therefore given by:

$$Z_G(x_1, x_2, x_3, x_4, x_5) = \frac{1}{60} (x_1^{32} + 24x_1^2x_5^6 + 20x_1^2x_3^{10} + 15x_2^{16}).$$

Applying PET with weights $B = \text{black}$ and $W = \text{white}$ gives the CGF

$$\begin{aligned}
F(B, W) &= Z_G(B + W, B^2 + W^2, \dots, B^5 + W^5) \\
&= \frac{1}{60}((B + W)^{32} + 24(B + W)^2(B^5 + W^5)^6 + 20(B + W)^2(B^3 + W^3)^{10} + \\
&\quad 15(B^2 + W^2)^{16}) \\
&= B^{32} + 2B^{31}W + 13B^{30}W^2 + 86B^{29}W^3 + 636B^{28}W^4 + 3362B^{27}W^5 + \\
&\quad 15263B^{26}W^6 + 56130B^{25}W^7 + 175775B^{24}W^8 + 467520B^{23}W^9 + \\
&\quad 1076382B^{22}W^{10} + 2150460B^{21}W^{11} + 3765292B^{20}W^{12} + 5789700B^{19}W^{13} + \\
&\quad 7860190B^{18}W^{14} + 9428804B^{17}W^{15} + 10021408B^{16}W^{16} + 9428804B^{15}W^{17} + \\
&\quad 7860190B^{14}W^{18} + 5789700B^{13}W^{19} + \mathbf{3765292B^{12}W^{20}} + 2150460B^{11}W^{21} + \\
&\quad 1076382B^{10}W^{22} + 467520B^9W^{23} + 175775B^8W^{24} + 56130B^7W^{25} + \\
&\quad 15263B^6W^{26} + 3362B^5W^{27} + 636B^4W^{28} + 86B^3W^{29} + 13B^2W^{30} + \\
&\quad 2BW^{31} + W^{32}.
\end{aligned}$$

Reading off the coefficient of the term $B^{12}W^{20}$ gives 3,765,292 different ways to color the truncated icosahedron such that 12 faces are black and 20 faces are white.

To find the general formula for the distinct n -colorings of the truncated icosahedron under rotations, we simply substitute n into the cycle index:

$$Z_G(n, n, \dots, n) = \frac{1}{60} (n^{32} + 15n^{16} + 20n^{12} + 24n^8).$$

The total number of different 2-colorings is thus given by

$$\frac{1}{60}(2^{32} + 15 \cdot 2^{16} + 20 \cdot 2^{12} + 24 \cdot 2^8) = 71,600,640.$$

6.2 Number Theory

In number theory PET has been used to generalize various famous theorems, including those of Wilson, Gauss, Fermat and Euler. This work was done by Chong-Yun Chao and published in the Journal of Number Theory in 1982 [1].⁴ A generalization of both Fermat's theorem and Gauss' theorem is presented in this section.

The theorems of Fermat and Gauss are stated as follows:

Theorem 6.5. (Fermat's Little Theorem) If p is prime and p does not divide a , then

$$a^{p-1} \equiv 1 \pmod{p}. \quad (6.6)$$

If p is prime, then for every integer a

$$a^p \equiv a \pmod{p}. \quad (6.7)$$

⁴ Chao used a generalization of PET known as De Bruijn's Theorem.

Theorem 6.6. (Gauss' Theorem) If n is a positive integer, then

$$\sum_{d|n} \phi(d) = n. \quad (6.8)$$

These theorems are both generalized in the following theorem:

Theorem 6.7. Let a and n be positive integers. Then

$$\sum_{d|n} \phi(d)a^{n/d} \equiv 0 \pmod{n}. \quad (6.9)$$

Proof. Let $X = \{1, \dots, n\}$, $Y = \{1, \dots, a\}$ and let the cyclic group C_n act on X . Now if we assign the weight $w(y) = 1$ to each element in Y , by PET we get the CGF:

$$Z_{C_n}(a, a, \dots, a) = \frac{1}{n} \sum_{d|n} \phi(d)a^{n/d}. \quad (6.10)$$

Since the CGF gives the total number of configurations, which is a positive integer, we know that the RHS of 6.10 is a positive integer. It follows that

$$\sum_{d|n} \phi(d)a^{n/d} \equiv 0 \pmod{n}.$$

□

Example 6.8. If $a = 3$ and $n = 8$, then we have

$$\begin{aligned} \sum_{d|8} \phi(d)3^{8/d} &= \phi(1)3^8 + \phi(2)3^4 + \phi(4)3^2 + \phi(8)3 \\ &= 6672 = 8 \cdot 834 \equiv 0 \pmod{8}. \end{aligned}$$

Now we show how Fermat's Little Theorem follows from theorem 6.7. Letting p be a prime and $n = p$ in theorem 6.7 means

$$\frac{1}{p} \sum_{d|p} \phi(d)a^{p/d} = \frac{1}{p} (\phi(1)a^p + \phi(p)a) = \frac{1}{p} (a^p - a) + a \quad (6.11)$$

is a positive integer, say k . It follows that $a^p - a = (k - a)p$, i.e. $a^p \equiv a \pmod{p}$, which is equation 6.7. If a and p are relatively prime, then it also holds that $a^{p-1} \equiv 1 \pmod{p}$, which is equation 6.6. This is precisely Fermat's Little Theorem.

Gauss' theorem is also a simple consequence of theorem 6.7. Letting $a = 1$ in equation 6.10 gives

$$\sum_{d|n} \phi(d) \equiv 0 \pmod{n}.$$

This means that for some positive integer k we have

$$\frac{1}{n} \sum_{d|n} \phi(d) = k.$$

Since $a = 1$, there is only one possible configuration on Y^X , so $k = 1$. Thus

$$\sum_{d|n} \phi(d) = n$$

which is equation 6.8 and theorem 6.6 holds.

6.3 Graph Theory

The first application of Pólya's enumeration theorem was in graph theory. Pólya himself treated his 1937 paper as a continuation of Cayley's work on the enumeration of trees.[7] Since then, PET has been applied to enumerate many types of graphs with specified conditions. Some of these include labeled, rooted, connected, bipartite, and eulerian graphs, along with rooted trees, free trees, and tree-like structures.[4] In this section we present how PET has been used in enumerating isomorphism classes of rooted trees and (v,e)-graphs. Many of the enumeration techniques for specific types of trees or graphs depend on, or are variations of, these two results.[4]

6.3.1 Isomorphism Classes of Rooted Trees

Trees are connected graphs which do not contain cycles. The order p of a tree is the number of vertices in the tree. The number of edges stemming from a vertex is known as the degree of the vertex. In a rooted tree, one of the vertices is designated as the root. The tree is said to be labeled if each of its vertices has associated with it a unique positive integer less than or equal to p . Otherwise it is said to be unlabeled. Cayley proved that the number of labeled rooted p -trees is given by p^{p-2} .[4] The case of unlabeled p -trees, however, is much more difficult. We seek a generating function $T(x)$ which enumerates the non-isomorphic unlabeled rooted trees, i.e.

$$T(x) = \sum_{p=0}^{\infty} T_p x^p \tag{6.12}$$

where T_p is the number of rooted trees of order p . The first few rooted trees are listed below in figure 6.2 .

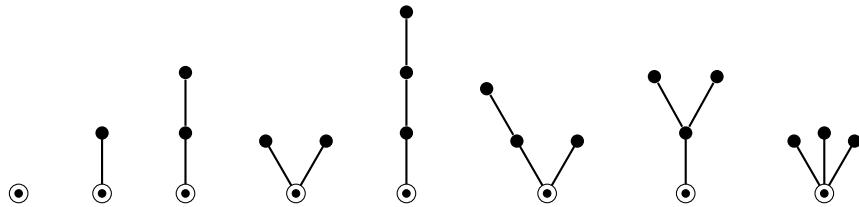


Fig. 6.2: The rooted trees up to order 3.

We begin by enumerating the rooted trees which have a root of degree n . Given a set with n rooted trees, a new rooted tree can be formed by adding a vertex and joining it to the roots of the trees in the set of n rooted trees. This new tree has a root with degree n . The symmetric group S_n can then be used to permute the n subtrees stemming from the new root. Figure 6.3 illustrates this method of generating new rooted trees. All trees with a root of degree n can clearly be formed in this manner.



Fig. 6.3: Forming a new rooted tree from a set of 3 rooted trees.

In order to enumerate the trees with a root of degree n we let $X = \{1, \dots, n\}$ and Y be the set of all rooted trees.⁵ To each rooted tree in Y we assign its weight to be x^k , where k is the number of vertices it contains. Summing over all weights of elements in Y yields $T(x)$. Thus applying PET gives the CGF as a recursive formula $T(x) = Z_{S_n}(T(x), T(x^2), T(x^3), \dots)$, where the coefficients of each x^k gives the number of trees with $k + 1$ vertices and a root of degree n . Multiplying through by x accounts for the new roots. Then summing over all n gives

$$T(x) = x \sum_{n=1}^{\infty} Z_{S_n}(T(x), T(x^2), T(x^3), \dots) \quad (6.13)$$

The following recursive formula for T_{p+1} in terms of T_1, \dots, T_p can then be derived using equation 6.13 and various identities:⁶

⁵ PET can be formulated to allow an infinite set of 'colors'.[4]

⁶ For details of derivations see [4, p.52-54]

$$T_{p+1} = p^{-1} \sum_{k=1}^p \left(\sum_{d|k} d T_d \right) T_{p-k+1} \quad (6.14)$$

The first 26 values of T_p are given by Harary and Palmer in [4, Appendix I]:⁷

p	T_p	p	T_p	p	T_p
1	1	10	719	19	4 688 676
2	1	11	1 842	20	12 826 228
3	2	12	4 766	21	35 221 832
4	4	13	12 486	22	97 055 181
5	9	14	32 973	23	268 282 855
6	20	15	87 811	24	743 724 984
7	48	16	235 381	25	2 067 174 645
8	115	17	634 847	26	5 759 636 510
9	286	18	1 721 159		

Tab. 6.1: The number of rooted trees with p vertices.

6.3.2 Isomorphism Classes of (v,e) Graphs

A (v, e) graph is a graph with v vertices and e edges. Two (v, e) graphs are said to be isomorphic if there is an edge-preserving bijection between them. We seek a generating function $G_v(x)$ with the coefficient of each x^e giving the number of non-isomorphic (v, e) graphs $g_{v,e}$, i.e.

$$G_v(x) = \sum_{e=0}^{\binom{v}{2}} g_{v,e} x^e. \quad (6.15)$$

We let V be the set of v vertices, and $V^{(2)}$ be the set of all possible 2-subsets, or edges, of V . Two graphs G and G' with v vertices are isomorphic if a permutation of the vertices exists that maps the edges of G to the edges of G' . The symmetric group S_v is the appropriate permutation group on the vertices of a graph and it induces a natural group of permutations $S_v^{(2)}$ on the edges known as the *pair group* of S_v . An element $\sigma \in S_v$ induces the element $\sigma' \in S_v^{(2)}$ by the equation

$$\sigma'(x, y) = (\sigma(x), \sigma(y)), \text{ for each } (x, y) \in V^{(2)}.$$

The pair group $S_v^{(2)}$ thus acts on the set of edges $V^{(2)}$, and two graphs are isomorphic if and only if there exists a permutation in $S_v^{(2)}$ that maps the edges of one graph to the

⁷ The sequence is also found in the OEIS as sequence A000081.

edges of the other. Let Y be the set with two colors *black* and *white* with weights B and W respectively. Functions in $Y^{V^{(2)}}$ map possible edges of the graph either to *black* or *white*. Thus once we have used PET to enumerate the distinct 2-colorings of the edges of the complete v -graph, we may interpret black edges as present and white edges as absent, hence giving the number of distinct graphs on v vertices. The configuration generating function for the non-isomorphic graphs with white and black edges is thus:

$$F(B, W) = Z_{S_v^{(2)}}(W + B, W^2 + B^2, \dots, W^{\binom{v}{2}} + B^{\binom{v}{2}}) \quad (6.16)$$

where the cycle index of the pair group of the symmetric group with v elements is given by Harary and Palmer in [4, p.84] as:⁸

$$Z_{S_v^{(2)}}(x_1, x_2, \dots) = \sum_{(j)} \frac{1}{\prod k^{j_k} j_k!} \prod_k x_{2k+1}^{kj_{2k+1}} \prod_k (x_k x_{2k}^{k-1})^{j_{2k}} x_k^{k \binom{j_k}{2}} \prod_{r < t} x_{lcm(r,t)}^{gcd(r,t)j_r j_t} \quad (6.17)$$

where the sum is taken over the partitions $(j) = (j_1, j_2, \dots, j_k, \dots, j_v)$ of v .

Since $F(B, W)$ gives a polynomial with variables B and W , but we are not interested in white (absent) edges, we may assign the value 1 to W , which leaves all other values in the CGF unaltered. Thus the generating function 6.15 is given by substituting $W = 1$ and $B = x$ in 6.16, i.e.

$$G_v(x) = F(x, 1) = Z_{S_v^{(2)}}(1 + x, 1 + x^2, \dots, 1 + x^{\binom{v}{2}}). \quad (6.18)$$

We demonstrate the case $v = 5$ in the following example:

Example 6.9. *We use PET to enumerate the isomorphism classes of $(5, e)$ graphs. First we find the cycle index. The number 5 can be partitioned in seven ways, namely $1 + 1 + 1 + 1 + 1$, $1 + 1 + 1 + 2$, $1 + 1 + 3$, $1 + 2 + 2$, $1 + 4$, $2 + 3$ and 5 . Thus the possible values for partitions $(j) = (j_1, j_2, j_3, j_4, j_5)$ are:*

$$\begin{array}{lll} (5, 0, 0, 0, 0) & (3, 1, 0, 0, 0) & (2, 0, 1, 0, 0) \\ (1, 2, 0, 0, 0) & (1, 0, 0, 1, 0) & (0, 1, 1, 0, 0) \\ & (0, 0, 0, 0, 1) \end{array}$$

Now by somewhat tedious calculations using equation 6.17 we can find the monomial which $(5, 0, 0, 0, 0)$ contributes to the cycle index. First we note that $j_1 = 5$ and $j_k = 0$

⁸ The cycle index given in [4, p.84] contained an extra factor $v!$ which was cancelled out and is thus not visible in equation 6.17.

when $k \neq 1$. Thus

$$\begin{aligned} \frac{1}{\prod k^{j_k} j_k!} &= \frac{1}{(1^5 5!)(2^0 0!)(3^0 0!)(4^0 0!)(5^0 0!)} = \frac{1}{(1^5 5!)} \\ \prod_k x_{2k+1}^{k j_{2k+1}} &= (x_3^{1 \cdot 0})(x_5^{2 \cdot 0})(x_7^{3 \cdot 0})(x_9^{4 \cdot 0})(x_{11}^{5 \cdot 0}) = 1 \\ \prod_k (x_k x_{2k}^{k-1})^{j_{2k}} x_k^{k \binom{j_k}{2}} &= ((x_1 x_2^0)^0 x_1^{1 \cdot \binom{5}{2}}) \cdot ((x_2 x_4^1)^0 x_2^{2 \cdot \binom{0}{2}}) \cdot ((x_3 x_6^2)^0 x_3^{3 \cdot \binom{0}{2}}) \cdot \\ &\quad ((x_4 x_8^3)^0 x_4^{4 \cdot \binom{0}{2}}) \cdot ((x_5 x_{10}^4)^0 x_5^{5 \cdot \binom{0}{2}}) = x_1^{\binom{5}{2}} \\ \prod_{r < t} x_{lcm(r,t)}^{gcd(r,t)j_r j_t} &= (x_{lcm(1,2)}^0)(x_{lcm(1,3)}^0)(x_{lcm(2,3)}^0)(x_{lcm(1,4)}^0) \cdots (x_{lcm(4,5)}^0) = 1 \end{aligned}$$

Hence the partition $(5, 0, 0, 0, 0)$ contributes to the cycle index the term:

$$\frac{1}{1^5 5!} (1) (x_1^{\binom{5}{2}}) (1) = \frac{1}{120} x_1^{10}$$

Similarly $(3, 1, 0, 0, 0)$ contributes the term:

$$\frac{1}{1^3 3! 2^1 1!} (x_3^0 x_5^0) ((x_1 x_2^0)^1 x_1^{\binom{3}{2}} (x_2 x_4)^0 x_2^{2 \cdot \binom{1}{2}}) (x_{lcm(1,2)}^{3 \cdot gcd(1,2)}) = \frac{1}{12} x_1^4 x_2^3$$

$(2, 0, 1, 0, 0)$ contributes the term:

$$\frac{1}{3^1 1! 1^2 2!} (x_3^1) (x_1 x_2^0)^0 x_1^{\binom{2}{2}} (x_2 x_4)^0 x_2^{\binom{0}{2}} (x_{lcm(1,3)}^{2 \cdot gcd(1,3)}) = \frac{1}{6} x_1 x_3^3$$

$(1, 2, 0, 0, 0)$ contributes the term:

$$\frac{1}{1^1 1! 2^2 2!} (x_3^0 x_5^0) (x_1 x_2^0)^2 x_1^{\binom{1}{2}} (x_2 x_4^3)^0 x_2^{2 \binom{2}{2}} (x_{lcm(1,2)}^{gcd(1,2) \cdot 2}) = \frac{1}{8} x_1^2 x_2^4$$

$(1, 0, 0, 1, 0)$ contributes the term:

$$\frac{1}{1^1 1! 4^1 1!} (x_3^0 x_5^0) (x_1 x_2^0)^0 x_1^{\binom{1}{2}} (x_2 x_4)^1 x_4^{4 \binom{1}{2}} (x_{lcm(4,1)}^{gcd(4,1)}) = \frac{1}{4} x_2 x_4^2$$

$(0, 1, 1, 0, 0)$ contributes the term:

$$\frac{1}{2^1 1! 3^1 1!} (x_3^1) (x_1 x_2^0)^1 x_1^{\binom{0}{2}} (x_2 x_4^1)^0 (x_2)^2 \binom{1}{2} (x_{lcm(2,3)}^{gcd(2,3)}) = \frac{1}{6} x_1 x_3 x_6$$

$(0, 0, 0, 0, 1)$ contributes the term:

$$\frac{1}{5^1 1!} (x_5)^2 (x_5^{5 \binom{1}{2}}) (1) = \frac{1}{5} x_5^2$$

The cycle index is thus given by:⁹

$$Z_{S_5^{(2)}} = \frac{1}{120} (x_1^{10} + 10x_1^4x_2^3 + 20x_1x_3^3 + 15x_1^2x_2^4 + 30x_2x_4^2 + 20x_1x_3x_6 + 24x_5^2)$$

Now by equation 6.18 we have

$$\begin{aligned} G_5(x) &= Z_{S_5^{(2)}}(1+x, 1+x^2, \dots, 1+x^6) \\ &= \frac{1}{120} \left((1+x)^{10} + 10(1+x)^4(1+x^2)^3 + 20(1+x)(1+x^3)^3 + \right. \\ &\quad 15(1+x)^2(1+x^2)^4 + 30(1+x^2)(1+x^4)^2 + \\ &\quad \left. 20(1+x)(1+x^3)(1+x^6) + 24(1+x^5)^2 \right) \\ &= 1 + x + 2x^2 + 4x^3 + 6x^4 + 6x^5 + 6x^6 + 4x^7 + 2x^8 + x^9 + x^{10} \end{aligned}$$

The coefficients of each x^e in $G_5(x)$ now gives the number of $(5, e)$ graphs. For example, there are 6 non-isomorphic $(5, 5)$ graphs. The total number of non-isomorphic $(5, e)$ graphs is $G_5(1) = 34$. These are listed in figure 6.4, where each column has the same number of edges.

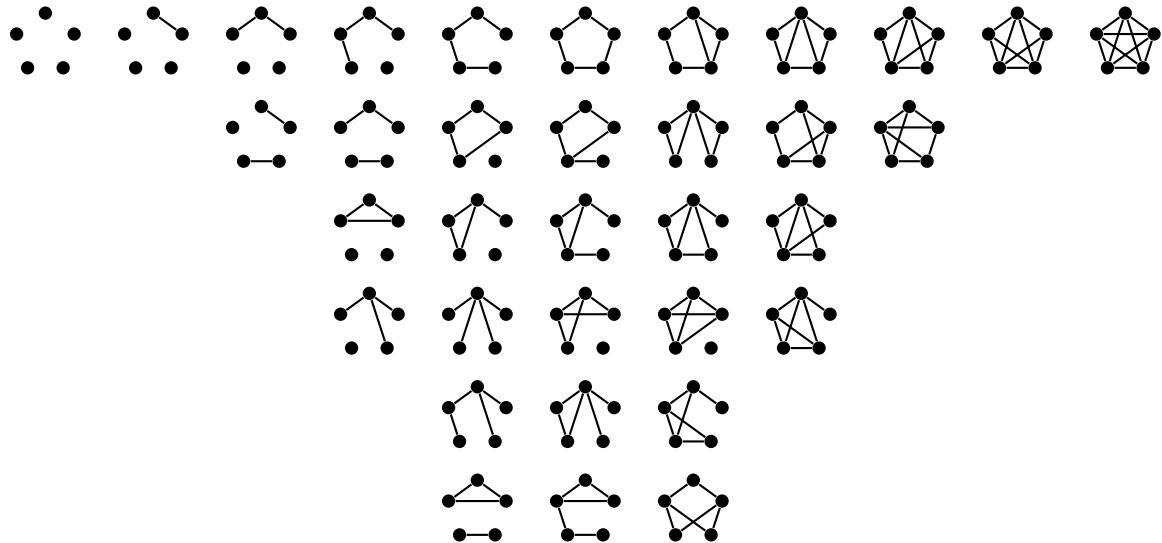


Fig. 6.4: Isomorphism classes of $(5, e)$ graphs.

6.4 Enumeration of Chemical Compounds

The applications of graphical enumeration in theoretical chemistry have been known since the time of Cayley. In fact, the chemical interpretations of graph theory were

⁹ This matches the result of Harary and Palmer, who provided the cycle indices of pair groups $S_n^{(2)}$ for $n \leq 10$ in [4, Appendix III].

largely what motivated his research in the enumeration of trees. Pólya, continuing in Cayley's footsteps, spent a considerable amount of his groundbreaking 1937 paper on the applications of PET in chemical enumeration.[7]

In chemistry, there is generally no bijective correspondence between the set of molecules and the set of chemical formulas. A chemical formula may represent more than one molecule, whose arrangement of atoms differs in space. Such molecules with the same chemical formula but different chemical structures are known as isomers. PET can be used to enumerate different types of isomers.[7]

Example 6.10. *A simple example is finding the isomers of dichlorobenzene $C_6H_4Cl_2$. The dichlorobenzene molecule is formed by replacing two hydrogen atoms in the benzene ring C_6H_6 with chlorine atoms.*



Fig. 6.5: The chemical structures of a benzene ring and the three dichlorobenzene isomers.

The number of ways of attaching two chlorine atoms and four hydrogen atoms to the ring of carbons is identical to a necklace coloring problem using two colors. We assign $X = \{1, 2, \dots, 6\}$ to be the six corners of the hexagon, Y the set containing a chlorine atom and hydrogen atom with weights $w(\text{chlorine}) = Cl$ and $w(\text{hydrogen}) = H$. The appropriate group acting on X is clearly the cyclic group C_6 . Applying PET gives the configuration generating function:

$$\begin{aligned}
 F(H, Cl) &= Z_{C_6}(H + Cl, H^2 + Cl^2, \dots, H^6 + Cl^6) \\
 &= \frac{1}{6} \left((H + Cl)^6 + (H^2 + Cl^2)^3 + 2(H^3 + Cl^3)^2 + 2(H^6 + Cl^6) \right) \\
 &= H^6 + H^5Cl + 3H^4Cl^2 + 4H^3Cl^3 + 3H^2Cl^4 + HCl^5 + Cl^6
 \end{aligned}$$

The coefficient of H^4Cl^2 shows that there are three isomers of dichlorobenzene. These were listed in Figure 6.5.

Next we present a more complicated example given by Pólya in [7].

Example 6.11. *A cyclopropane molecule C_3H_6 is formed from three carbon atoms joined by double bonds and six hydrogen atoms which attach to each of the carbon atoms in pairs. The three dimensional chemical structure is shown in Figure 6.6.*

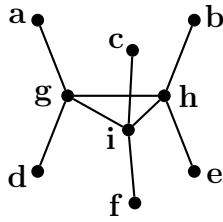


Fig. 6.6: Structure of Cyclopropane Molecule

The hydrogen atoms may be replaced by monovalent radicals, which are molecules with a free bond that may be treated as a single atom.¹⁰ The resulting molecules are known as derivatives of cyclopropane.

Pólya identifies three chemically relevant groups that can act on the vertices of the graph of cyclopropane in Figure 6.6. The first is the group G_1 of spatial rotations of the graph in three dimensions. The group of symmetries is the same as that of a regular prism rotated in three dimensions. Pólya coined this the “group of the stereoformula” and gave its cycle index:

$$Z_{G_1}(x_1, x_2, x_3) = \frac{1}{6} (x_1^6 + 3x_2^3 + 2x_3^2)$$

This is easily verified. The prism has six vertices, which in figure 6.6 are labeled a, b, c, d, e and f . Now $G_1 = \{(a)(b)(c)(d)(e)(f), (abc)(def), (cba)(fed), (ad)(bf)(ce), (ae)(bd)(cf), (af)(cd)(be)\}$. From the group structure we can see directly that the cycle index holds.

The second permutation group G_2 is the group of spatial rotations and reflections of the cyclopropane graph. This group includes the six mirror images of the prism, resulting in a total of 12 permutations. Pólya called it the “extended group of the stereoformula” and gave its cycle index:

$$Z_{G_2}(x_1, x_2, \dots, x_6) = \frac{1}{12} (x_1^6 + 4x_2^3 + 2x_3^2 + 3x_1^2x_2^2 + 2x_6)$$

This is derived similarly to the cycle index of G_1 , using the fact that $G_2 = G_1 \cup \{(ad)(cf)(be), (aecdbf), (fbdccea), (a)(d)(bc)(ef), (b)(e)(ac)(df), (c)(f)(ab)(de)\}$.

The final group G_3 is the group of topologically congruent arrangements. The central triangle of carbon atoms (vertices g, h , and i in figure 6.6) can be arranged in 6 ways under the group action induced by S_3 , and the each of the radicals then in turn in 2 ways under the group action S_2 . Thus there are $2^3 = 8$ ways to arrange the three radicals, resulting in a total of $6 \cdot 8 = 48$ permutations in G_3 . The resulting group is equivalent to the group of 48 rotations and reflections of the vertices of the octahedron. This group

¹⁰ Some examples of monovalent radicals are $-OH$, $-C_1H_3$, and $-NO_3$.

was referred to by Pólya as the “group of the structural formula”. He derived it by substituting the cycle index of S_2 into the cycle index of S_3 , producing the cycle index:

$$\begin{aligned}
 Z_{G_3}(x_1, x_2, \dots, x_6) &= Z_{S_3}(Z_{S_2}(x_1, x_2), Z_{S_2}(x_2, x_4), Z_{S_2}(x_3, x_6)) \\
 &= \frac{1}{6}(Z_{S_2}(x_1, x_2)^3 + 3Z_{S_2}(x_1, x_2)Z_{S_2}(x_2, x_4) + 2Z_{S_2}(x_3, x_6)) \\
 &= \frac{1}{6}\left(\frac{1}{2}(x_1^2 + x_2)^3 + 3 \cdot \frac{1}{2}(x_1^2 + x_2) \cdot \frac{1}{2}(x_2^2 + x_4) + 2 \cdot \frac{1}{2}(x_3^2 + x_6)\right) \\
 &= \frac{1}{48}(x_1^6 + 3x_1^4x_2 + 9x_1^2x_2^2 + 6x_4x_1^2 + 7x_2^3 + 6x_4x_2 + 8x_3^2 + 8x_6)
 \end{aligned}$$

Now, for each type of symmetry, we can find the number of different derivatives of cyclopropane of the form $C_3X_kY_lZ_m$, where $k+l+m=6$ and X , Y and Z are different independent radicals.¹¹ Applying PET with the three cycle indices above and weights $w(X)=x$, $w(Y)=y$ and $w(Z)=z$ gives configuration generating functions:¹²

$$\begin{aligned}
 F_1(x, y, z) &= Z_{G_1}(x + y + z, x^2 + y^2 + z^2, x^3 + y^3 + z^3) \\
 &= x^6 + x^5y + x^5z + 4x^4y^2 + 5x^4yz + 4x^4z^2 + 4x^3y^3 + 10x^3y^2z + 10x^3yz^2 + \\
 &\quad 4x^3z^3 + 4x^2y^4 + 10x^2y^3z + 18x^2y^2z^2 + 10x^2yz^3 + 4x^2z^4 + xy^5 + 5xy^4z + \\
 &\quad 10xy^3z^2 + 10xy^2z^3 + 5xyz^4 + xz^5 + y^6 + y^5z + 4y^4z^2 + 4y^3z^3 + 4y^2z^4 + \\
 &\quad yz^5 + z^6
 \end{aligned}$$

$$\begin{aligned}
 F_2(x, y, z) &= Z_{G_2}(x + y + z, x^2 + y^2 + z^2, \dots, x^6 + y^6 + z^6) \\
 &= x^6 + x^5y + x^5z + 3x^4y^2 + 3x^4yz + 3x^4z^2 + 3x^3y^3 + 6x^3y^2z + 6x^3yz^2 + \\
 &\quad 3x^3z^3 + 3x^2y^4 + 6x^2y^3z + 11x^2y^2z^2 + 6x^2yz^3 + 3x^2z^4 + xy^5 + 3xy^4z + \\
 &\quad 6xy^3z^2 + 6xy^2z^3 + 3xyz^4 + xz^5 + y^6 + y^5z + 3y^4z^2 + 3y^3z^3 + 3y^2z^4 + \\
 &\quad yz^5 + z^6
 \end{aligned}$$

$$\begin{aligned}
 F_3(x, y, z) &= Z_{G_3}(x + y + z, x^2 + y^2 + z^2, \dots, x^6 + y^6 + z^6) \\
 &= x^6 + x^5y + x^5z + 2x^4y^2 + 2x^4yz + 2x^4z^2 + 2x^3y^3 + 3x^3y^2z + 3x^3yz^2 + \\
 &\quad 2x^3z^3 + 2x^2y^4 + 3x^2y^3z + 5x^2y^2z^2 + 3x^2yz^3 + 2x^2z^4 + xy^5 + 2xy^4z + \\
 &\quad 3xy^3z^2 + 3xy^2z^3 + 2xyz^4 + xz^5 + y^6 + y^5z + 2y^4z^2 + 2y^3z^3 + 2y^2z^4 + \\
 &\quad yz^5 + z^6
 \end{aligned}$$

Reading off the coefficients of the term x^4y^2 gives the number of different derivatives of cyclopropane of the form $C_3X_4Y_2$. There are four unique derivatives under spatial rotations, three unique derivatives if mirror images are disregarded, and two unique derivatives if spatial arrangement is disregarded.

¹¹ “Independent means that $X_kY_lZ_m$ and $X_{k'}Y_{l'}Z_{m'}$ have the same molecular structure only if $k=k'$, $l=l'$ and $m=m'$.⁷” [7]

¹² Pólya only gives the first few terms of each polynomial, the rest were calculated using Maple 2015.

7 Conclusion

In the previous chapter we saw the power and generality of Pólya’s Enumeration Theorem as it was applied to various different applications. Problems which would be extremely tedious using Burnside’s lemma, such as coloring the truncated icosahedron, were solved by PET with relative ease. The enumeration of unlabeled rooted trees was done by formulating PET into a recursive equation. The properties of the cycle index for the cyclic group proved to have connections to number theory.

Despite its generality, PET does have certain limitations. Often the main difficulty in applying it is finding the cycle index, as it can be something as unwieldy as for the pair group in equation 6.17. It is also not hard to pose problems which are seemingly Pólya type problems but cannot be solved by PET. For example, PET requires the choice of colors to be independent of one another, i.e. the choice of one color does not affect the choice of another. Given a necklace coloring problem using six beads and three colors, if we add the restriction that two adjacent beads cannot have the same color, then the colorings are no longer independent. This problem can no longer be solved by PET, but can in fact be done by resorting back to Burnside’s lemma. PET has been generalized further, and a notable such generalization was done by De Bruijn in 1959. Considering again example 6.3, we have the group of rotations G acting on the set of faces of the cube X , and the set of colors Y . Suppose now that we consider two colorings equivalent not only if one can be obtained from the other by rotations, but also if it can be obtained by interchanging the colors of the faces. Thus in addition to G acting on X , we have a group H acting on the set of colors Y . In such a situation De Bruijn’s generalization can be used to enumerate the configurations.[7]

Limitations and generalizations aside, PET itself solved a whole class of enumeration problems in a single unifying theorem, making a significant contribution to combinatorial mathematics. With its wide range of applications, PET has proved to be a valuable tool in the discrete mathematician’s toolbox.

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