Pólya's One Theorem with 100 Pages of Applications

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B Sury has been with the ISI, Bangalore since 1999. Apart from his interest in teaching mathematics at the undergraduate level, he has also long-standing interest in the mathematical olympiad programme in the country.
He would like to introduce this article on Pólya by:

Believe me, Mathematics is an asset
in counting (it can aid and abet)
of different isomers – even stereo.
We'd have bid it cheerio
but for this magic PET !

In 1937, George Pólya wrote what is considered one of the most significant papers in 20th-century mathematics. The article contained one theorem and 100 pages of applications. It introduced a combinatorial method which led to unexpected applications to diverse problems in science like the enumeration of isomers of chemical compounds. Pólya's theory of enumeration was discussed in detail in [1] by Shriya Anand, a summer student of the author. In what follows, we briefly recall the theory and complement the earlier article by adding some other applications not discussed there.

We start with an example. Consider the problem of painting each face of a cube either black or white. How many such distinct colourings are there? Since the cube has 6 faces, and we have 2 colours to choose from, the number of possible colourings is 2^6. However, painting the top face white and all other faces black produces the same pattern as painting the bottom face white and all other faces black, as we can invert the cube and it looks the same! The answer to the above question is thus not so obvious. To find the various possible colour patterns which are inequivalent, we exploit the fact that the rotational symmetries of the cube have the structure of a group.

Before explaining how the above problem is dealt with in more precise terms by Pólya's theory, we mention that the scope of Pólya's theory is extraordinarily wide because of its simple and general expression. This theory deals with the enumeration of mathematical configura-

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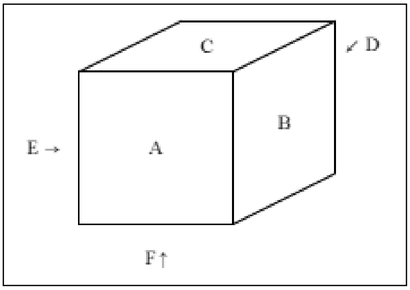

Figure 1.

tions which can be thought of as placement of shapes in receptacles. More abstractly, we have mappings from a set D of 'receptacles' to a set R of 'shapes'. Thus, in a configuration, two elements of D may have the same image in R; that is, the same shape can be placed in more than one receptacle. Each shape is given a value, and the value of a configuration is the total value of all the shapes. A typical problem would be to determine the number of configurations with a given value. Permutations of the receptacles which yield configurations equivalent to the original one give rise to a group, and the theory is stated in terms of this group. For instance, in the cube-colouring problem, let D be the set of 6 faces of the cube, and R the set of two colours: black and white. A configuration here is a colouring of the faces by the two colours; that is, a mapping $\phi : D \to R$.

The group of rotations of the 6 faces has 24 elements: (i) the identity element; (ii) rotations about the lines joining centres of opposite faces like $\{\mathrm{A}, \mathrm{D}\}$ in *Figure* 1, through 90°, 180° and 270° respectively (there are $3 \times 3 = 9$ such rotations); (iii) rotations by 180° about lines joining the centers of diagonally opposite edges (there are $12/2 = 6$ such rotations); (iv) rotations about the main diagonals of the cube, through 120° and 240° respectively ($4 \times 2 = 8$ such rotations). To avoid ambiguity, all rotations here have a clockwise sense.

Returning to the cube-colouring problem, let X be the set of all colourings. With respect to the group G of permutations of D, we define an equivalence of elements in X as follows:

$\phi_1 \sim \phi_2$ if, and only if, there exists some $g \in G$ such that $\phi_1 g = \phi_2$.

As G is a group, $\sim$ is an equivalence relation on X. Hence it partitions X into disjoint equivalence classes. It is clear that the orbits of the action, i.e., the equivalence classes under $\sim$, are precisely the different colour patterns. Therefore, we need to find the number of orbits of the action of G on X. Pólya's theorem has as its starting point a lemma known popularly as Burnside's lemma although it was already known due to Cauchy and Frobenius. It says that for a group G of transformations on a set X, the number of orbits is $\frac{1}{|G|}\sum_{g \in G}|X^g|$ where X^g is the set of points of X fixed by g. In the problem of colouring cubes with two colours, the lemma suffices to find the number of configurations. We describe this now. Finer information like how many configurations have 2 white faces and 4 black faces need the force of Pólya's theorem.

In the cube-colouring problem with two colours, X has 2^6 elements. Let us see how the above-mentioned 24 transformations affect X. The identity, of course, fixes all 2^6 elements of X. Now consider the rotations in (ii): if the angle of rotation is 90°, they fix all those colourings where faces $\{\mathrm{B, C, E, F}\}$ have the same colour and $\{\mathrm{A, D}\}$ are arbitrarily coloured. Likewise for rotations through 270°. For rotations through 180°, the colours of $\{\mathrm{B, E}\}$ should match, as should the colours of $\{\mathrm{C, F}\}$. The transformations in (ii) fix those colourings where $\{\mathrm{A, B}\}$ have the same colour, $\{\mathrm{D, E}\}$ have the same colour, and $\{\mathrm{C, F}\}$ have the same colour. Under the transformations of type (iv), a colouring which is fixed must have three 'top' faces of the same colour and three 'bottom' faces of the same colour. Thus, the sum $\sum_{g \in G}|X^g|$ equals

$$2^6 + 6 \cdot 2^3 + 8 \cdot 2^2 + 3 \cdot 2^2 \cdot 2^2 + 6 \cdot 2^2 \cdot 2 = 240.$$

By the Cauchy–Frobenius–Burnside lemma, the number

The well-known `Burnside lemma' was already known to Cauchy and Frobenius. Peter Neumann wrote an amusing note titled ` A lemma that is not Burnside's'.

of orbits is $240/24 = 10$.

To describe Pólya's theorems, we consider only finite sets D, R like in the example of the cube. For a group G of permutations on a set of n elements and variables $s_1, s_2, \ldots, s_n$, one defines a polynomial expression (called the cycle index) for each $g \in G$. If $g \in G$, let $\lambda_i(g)$ denote the number of i-cycles in the disjoint cycle decomposition of g. Then, the cycle index of G, denoted by $z(G; s_1, s_2, \ldots, s_n)$ is defined as the polynomial expression

$$z(G; s_1, s_2, \ldots, s_n) = \frac{1}{|G|} \sum_{g \in G} s_1^{\lambda_1(g)} s_2^{\lambda_2(g)} \ldots s_n^{\lambda_n(g)}.$$

For instance,

$$z(S_n; s_1, s_2, \ldots, s_n) = \sum_{\lambda_1 + 2\lambda_2 + \ldots + k\lambda_k = n} \frac{s_1^{\lambda_1} s_2^{\lambda_2} \ldots s_k^{\lambda_k}}{1^{\lambda_1} \lambda_1! 2^{\lambda_2} \lambda_2! \ldots k^{\lambda_k} \lambda_k!}.$$

We may view the above-mentioned configurations obtained by placing a set R of shapes in D receptacles also as a colouring problem: the shapes can be thought of as colours, and the receptacles as various objects to be coloured. Here is Pólya's theorem:

Theorem (Pólya). *Suppose D is a set of m objects to be coloured using a range R of k colours. Let G be the group of symmetries of D. Then, the number of colour patterns is*

$$\frac{1}{|G|} z(G; k, k, \ldots, k).$$

The cycle index of the group G of symmetries of the 6 faces of the cube turns out to be

$$z(G; s_1, \cdots, s_6) = \frac{1}{24}(6s_1^2 s_4 + 3s_1^2 s_2^2 + 8s_3^2 + 6s_2^3 + s_1^6).$$

So, in our example of the cube, the number of distinct colourings of the cube is:

$$\frac{1}{24}\left(2^6 + 6 \cdot 2^3 + 8 \cdot 2^2 + 3 \cdot 2^2 \cdot 2^2 + 6 \cdot 2^2 \cdot 2\right) = 10.$$

The group of symmetries of the six vertices of a regular octahedron is the same as the group of symmetries of the six faces of the cube.

So, using two colours, there are 10 distinct colourings of the cube, as we saw above.

Incidentally, if we look at a regular octahedron, then the group of symmetries of the 6 *vertices* is the same group above of symmetries of the 6 *faces* of the cube!

A 'Valuable' Version of Pólya's Theorem

The above version of Pólya's theorem gives us the total number of configurations but we can retrieve finer information from other versions. We look at one example before proceeding to some other applications of Pólya's theorem. As mentioned earlier, one could assign a value for each shape/colour in R and enumerate the number of configurations with a given value. It is convenient to constrain values of shapes to be non-negative integers. One forms the generating function

$$c(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + \cdots$$

which is a polynomial, where c_k is the number of shapes with value k. The finer version of Pólya's theorem we are alluding to asserts that if a_k is the number of configurations with total value k, then the generating function

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots ,$$

is obtained by substituting $c(x^r)$ for s_r in the cycle index.

For simplicity, suppose R has two elements black and white which have values 0 and 1. Then, the generating polynomial above is simply $1 + x$.

Let us discuss the example of chlorination of benzene where some hydrogen atoms get substituted by chlorine atoms. Assign the values 0 and 1 to Cl and H, and note that the group of symmetries of the benzene molecule is the group of rotations of the regular hexagon, which is the dihedral group D_6 of order 12. The cycle index of D_6 is

$$z(D_6) = \frac{1}{12}\left(s_1^6 + 4s_2^3 + 2s_3^2 + 3s_1^2 s_2^2 + 2s_6\right).$$

Substituting $1 + x^r$ for s_r's, we obtain the polynomial

$$\frac{1}{12}\Big((1+x)^6 + 4(1+x^2)^3 + 2(1+x^3)^2 + 3(1+x)^2(1+x^2)^2 + 2(1+x^6)\Big)$$
$$= 1 + x + 3x^2 + 3x^3 + 3x^4 + x^5 + x^6.$$

So the number of configurations with 2 chlorine atoms is the coefficient of x^4, which is 3. These are the ortho dichlo-robenzenes, meta dichlorobenzenes and para dichlorobenzenes where the gaps between the vertices corresponding to the carbon atoms to which the two chlorine atoms are attached are 1, 2 and 3 edges respectively.

Topologically different trees with n four-edged vertices and $2n + 2$ one-edged vertices correspond to the different isomers with the molecular formula C_nH_{2n+2}.

More general weighted versions of Pólya's theorem as well as the immediate applications to enumerating isomers of chemical compounds were discussed in detail in [1].

Enumeration of Graphs

A key application of Pólya's theorem is to the enumeration of graphs. Indeed, the introduction of Pólya's paper begins with the words (as translated by Read [2]):

> "This paper presents a continuation of work done by Cayley. Cayley has repeatedly investigated combinatorial problems regarding the determination of the number of certain trees. Some of his problems lend themselves to chemical interpretation: the number of trees in question is equal to the number of certain theoretically possible chemical compounds."

Indeed, a chemical compound with no multiple bonds corresponds to a tree where different types of vertices

Pólya named and used the so-called wreath product of groups as permutation groups. His paper gave the first precise definition but, interestingly, in 1845, A Cauchy had used this same notion somewhat vaguely in his proof of his famous result that there is an element of any given prime order dividing the order of a finite group. Cauchy's 1845 paper also was the first to use the notion of double cosets.

correspond to different atoms. In case of multiple bonds, one may regard different kinds of edges also.

A tree consists of vertices and edges and is a connected graph where each edge connects two vertices. There can be several edges meeting at a vertex. There is no closed path. Therefore, the number of edges is one less than the number of vertices. A vertex is called r-edged if there are exactly r edges originating there.

Consider an alkane; this has the formula C_nH_{2n+2}. The carbon atoms are usually assumed to have valency 4 which means that the structure of the alkane is determined (that is, the positions of the hydrogen atoms are uniquely determined) by the structure formed by the carbon atoms. Topologically different trees with n four-edged vertices and $(2n + 2)$ one-edged vertices correspond to the different isomers with the molecular formula C_nH_{2n+2}.

Thus, the enumeration of isomers as above is equivalent to the enumeration of trees as above. Interestingly, in Pólya's paper, he describes the groups of symmetries for certain chemical compounds as so-called 'wreath products'. Pólya calls wreath products as 'coronas'. As far as one can ascertain, this is the first introduction and study of finite wreath products as permutation groups.

Pólya's theorem was generalized by de Bruijn in a way which allows one to permute the shapes in R also.

Musings on Music

Pólya's theorem has been applied to the theory of music. One may determine the number of chords. To define this, one takes the n-scale to be the integers from 0 to $n-1$ under addition modulo n. There are translations $a \mapsto a + i$, where $0 \leq i < n$. An equivalence class (that is, an orbit) is called a chord, and one wishes to determine for each $r < n$, the number of r-chords; that is, the number of orbits consisting of r elements. This is equivalent to colouring the n-notes by two colours: we choose the notes in the chord by colouring them by one colour and those which are not in it by the other colour. The group is simply the cyclic group of order n whose cycle index is:

$$z(C_n; s_1, \cdots, s_n) = \frac{1}{n} \sum_{d|n} \phi(d) s_d^{n/d}.$$

In this, we substitute $1 + x^d$ for s_d and obtain the generating function whose coefficient of x^r is the number of r-chords. We obtain the number of r-chords to be

$$\frac{1}{n} \sum_{d|(n,r)} \phi(d) \binom{n/d}{r/d}.$$

Sometimes, one allows for a bigger group of transformations of the scale by allowing inversion $a \mapsto -a$ also. Then, the group becomes the dihedral group D_n of order $2n$ formed by the translations and the transposition above. In this case, as we have the cycle index of D_n to be

$$z(D_n; s_1, \cdots, s_n) = \frac{1}{2n} \sum_{d|n} \phi(\frac{n}{d}) s_{n/d}^d + \frac{1}{4}(s_1^2 s_2^{\frac{n}{2}-1} + s_2^{\frac{n}{2}})$$

if n is even, and

$$z(D_n; s_1, \cdots, s_n) = \frac{1}{2n} \sum_{d|n} \phi(\frac{n}{d}) s_{n/d}^d + \frac{1}{2} s_1 s_2^{\frac{n-1}{2}}$$

if n is odd, we may determine the number of r-chords in this dihedral case to be:

$$\frac{1}{2n} \sum_{d|(n,r)} \phi(d) \binom{n/d}{r/d} + \frac{1}{2} \binom{[n/2]}{[r/2]}$$

if n is odd;

$$\frac{1}{2n} \sum_{d|(n,r)} \phi(d) \binom{n/d}{r/d} + \frac{1}{2} \binom{n/2}{r/2}$$

In 12-tone music with dihedral symmetry, the number of pentachords is found to be 38 quickly from Pólya's theorem.

Much of Pólya's work had already been anticipated in 1927 by J H Redfield.

if n, r are even; and

$$\frac{1}{2n}\sum_{d|(n,r)}\phi(d)\binom{n/d}{r/d}+\frac{1}{2}\binom{\frac{n}{2}-1}{[r/2]}$$

if n is even and r is odd.

For example, in 12-tone music with dihedral symmetry, the number of pentachords is found to be 38.

For more details, the interested reader should refer to [3].

The original paper of Pólya was in German and was translated by R C Read, and this appears in a book now (see [4]). Also, several interesting generalizations and applications are discussed in [5], which is now available in an Indian edition. In passing, we mention that it was pointed out to the mathematical community as late as 1960 by Frank Harary that Pólya's work had been anticipated in 1927 by J H Redfield [6]!

Suggested Reading

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[2] G Pólya and R C Read, *Combinatorial enumeration of groups, graphs, and chemical compounds*, Springer-Verlag, 1987.

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