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Applications of Polya's Enumeration Formula

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Abstract:

This essay purely aims to provide basic information related to Polya's Enumeration Theorem and its applications in three distinct fields: Chemistry, Music, and Simple graph. Each section access the theorem in various insights and perspectives, resulting in a mix of ideas without strictly deeper focus.

Keywords: Polya's Enumeration Theorem; Cycle Index; Isomers; Simple Graph; Chord

1. Introduction

(1)Chemistry: Different spatial arrangements between molecules and a single chemical formula can represent more than one molecule (isomers) . The number of specific isomers can be counted using Polya's enumeration theorem. In this essay, we explore this problem, providing both theoretical insights and a concrete example using (Poly)chlorobenzenes.

(2)Music: Polya's enumeration theorem can be applied in diverse goals in music. Determining a specific k-chord in a n-scale to, we can enumrate the number of equivalence class of k-chord when considering symmetries and other limitations, helping achieve goals in enumration of certain kinds of chord and other "musical objects". This essay will focus on exploring the number of distinct distinct traids in typical 12-scale tone considering different group action acted on 3-chord permutations.

(3)Simple Graph: Graph theory is essential to many branches of mathematics and computer science, ranging from algorithm design to network analysis. Counting the number of simple non-isomorphic graphs for a given number of vertices, n, is a fundamental problem in this discipline. In this essay, we explore this problem, providing both theoretical insights and a concrete example using n=4 vertices.

2. Concepts

(1)Cycle index

In combinatorial mathematics, Cycle Index is a multivariable polynomial whose structure allows us to simply read how a permutation set acts on the set from coefficients and indices. Specifically, the periodic index polynomial is defined by decomposing finite permutation into several intersecting loops (i.e. loops without common elements).

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Here, k represents the number of replaced points. For each permutation, its periodic indicator mononomial is a mononomial composed of variables (a_1, a_2, $a_3 \ldots a_n$), where the variable (a_k) corresponds to a cycle with a period length (k).

The average value of the periodic index single term in the permutation group G is the periodic index polynomial of the permutation group G. The expression is:

$$Z(G)=\frac{1}{|G|}\sum h_{a_1 a_2 \ldots a_k \ldots a_n} f_1^{a_1} f_2^{a_2} \cdots f_k^{a_k} \cdots f_n^{a_n},$$

In this expression, ($j_k(g)$) represents the number of times (a_k) in the cyclic decomposition of the mutation (g), that is, the number of cycles of length (k). (H) is the coefficient, indicating the number of permutations containing (a_k) (k) cycles in the group G. (F) Variables represent different cycle lengths. Periodic index polynomials can be used to enumerate the equivalence classes formed by the action of groups.

(2)Simple graph

A simple graph is a collection of vertices (or nodes) connected by edges. Two graphs are said to be isomorphic if there is a one-to-one correspondence between their vertices and edges such that the adjacency (connectivity) is preserved. In simpler terms, if one graph can be transformed into another by simply renaming its vertices without altering the structure, the two graphs are isomorphic.

3. Applications

(1)Application in Chemistry:

In chemistry and molecular physics, a point group is a group of symmetrical operations that keep molecules or ions unchanged. These symmetric operations include rotation, reflection and inversion. This concept is used to classify molecules according to the symmetrical properties of molecules, which helps to predict the physical and chemical behaviour of molecules. The following are some common point groups and their related symmetric elements:

1) C1: asymmetric elements.

2) C2: Contains a C2 axis.

3) C4v:

Example: Tetrafluoro carbon (CF4)

Symmetrical elements: 1. C4 axis: The C atoms in CF4 are in the centre, and the four fluorine atoms are evenly distributed on the vertex of a regular tetrahedron. After rotating 90 degrees, the position of the fluorine atom remains unchanged. 2. 4 C2 axes: These axes pass through the symmetrical plane of CF4, which are perpendicular to the C4 axis. 3. 4 vertical mirrors (σ_v): Each mirror passes through the C4 axis and is perpendicular to the C2 axis. 4. No horizontal mirror (σ_h): There is no horizontal mirror in the symmetry of CF4, which conforms to the characteristics of C4v point group.

4) D4h:

Example: Titanium tetrachloride (TiCl4)

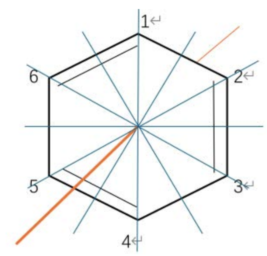
Symmetrical element: 1. C4 axis: In TiCl4, Ti atoms are located in the center, and four chlorine atoms are arranged on a square plane. After rotating 90 degrees, the position of the chlorine atom remains unchanged. 2. Four C2 axes: These C2 axes pass through different symmetric planes of molecules and are perpendicular to the C4 axis. 3. 4 vertical mirrors (σ_v): These mirrors pass through the C4 axis. 4. Horizontal mirror (σ_h): In TiCl4, the horizontal mirror on the molecular plane is symmetric.

5) T: The tetrahedral is symmetrical and consists of C3 and C2 axes.

6) O _ h: octahedral symmetry with multiple C3, C2 axes and mirror planes.

To determine the point group of the molecule, we need to check its symmetric elements and match them with the characteristics of the known point group. This classification helps to understand the vibration, spectral characteristics and reactivity of molecules.

Example of (Poly)chlorobenzenes



step a. Identify the point group

The basic benzene ring belongs to the (D_{6h}) point group. However, due to the presence of chiral ligands (chloride groups), the D6 group is enough to describe the arrangement characteristics of basic benzene ring. The symmetry characteristics of this point group can help us understand the symmetry of molecules.

step b. The next step involves determining the periodic index of D6 group. When applying each symmetric element in D6, getting the following arrangement:

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 1 & 2 & 3 & 4 & 5 & 6 \end{pmatrix}$$

E: = (1)([6^1]

300° = (1 2 3 4 5 6) 2)(3)(4)(5)(6) → [1^6]

$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 1 & 2 & 3 & 4 & 5 \end{pmatrix}$ C_6(orange):

60° = (1 6 5 4 3 2)

$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 4 & 5 & 6 & 1 \end{pmatrix} \rightarrow 2$

$\begin{pmatrix}1&2&3&4&5&6\\5&6&1&2&3&4\end{pmatrix}120° = (1\ 5\ 3)(2\ 6\ 4)$

$\rightarrow 2[3^2]$

$\begin{pmatrix}1&2&3&4&5&6\\3&4&5&6&1&2\end{pmatrix}240° = (1\ 3\ 5)(2\ 4\ 6)$

$\begin{pmatrix}1&2&3&4&5&6\\4&5&6&1&2&3\end{pmatrix}180° = (1\ 4)(2\ 5)(3\ 6) \quad \rightarrow [2^3]$

C_2(blue):

The midpoint of the opposite side

$\begin{pmatrix}1&2&3&4&5&6\\4&3&2&1&6&5\end{pmatrix}$56-23 (14)(23)(56) =

$\begin{pmatrix}1&2&3&4&5&6\\2&1&6&5&4&3\end{pmatrix}$12-45 (12)(36)(45) = $\rightarrow 3[2^3]$

$\begin{pmatrix}1&2&3&4&5&6\\6&5&4&3&2&1\end{pmatrix}$16-34 (16)(25)(34) =

Vertex

$\begin{pmatrix}1&2&3&4&5&6\\1&6&5&4&3&2\end{pmatrix}$1-4 (1)(4)(26)(35) =

$\begin{pmatrix}1&2&3&4&5&6\\3&2&1&6&5&4\end{pmatrix}$2-5 (2)(5)(13)(46) = $\rightarrow 3[1^2][2^2]$

$\begin{pmatrix}1&2&3&4&5&6\\5&4&3&2&1&6\end{pmatrix}$3-6 (3)(6)(15)(24) =

step c. Thus, the cycle index is

$$Z(D_6) = \frac{1}{12}\left(f_1^6 + 2f_6^1 + 2f_3^2 + f_2^3 + 3f_2^3 + 3f_1^2 f_2^2\right)$$

$$= \frac{1}{12}\left(f_1^6 + 2f_6^1 + 2f_3^2 + 4f_2^3 + 3f_1^2 f_2^2\right)$$

step d. Generating Function:

1) Defining the figure counting series where the power n of Cl means that the basic benzene ring attack n chloride atoms, as well as 1 (Cl^0) means zero chloride atoms. In the Pólya's theorem, the generation function is obtained by replacing the variable f with a figure counting series. In our case, the f's terms are given by

$$f_n^m = (1^n + Cl^n)^m$$

$1^n = 1$

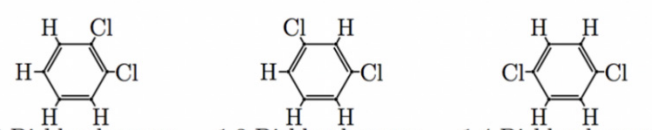
2) Now, substituting the figure counting into cycle index:

$$F(PCB) = \frac{1}{12}\Big[(1+Cl)^6 + 2(1+Cl^6) + 2(1+Cl^3)^2$$
$$+4(1+Cl^2)^3 + 3(1+Cl)^2(1+Cl^2)^2\Big]$$
$$= Cl^6 + Cl^5 + 3Cl^4 + 3Cl^3 + 3Cl^2 + Cl + 1$$

step e. Result

The coefficients of Cl to power of n indicate the number of isomers it has.

Example: The coefficient of 3H^4Cl^2 is 3, indicating there are three isomers. As the picture has shown:



1,2-Dichlorobenzene 1,3-Dichlorobenzene 1,4-Dichlorobenzene

(2)Application in Music

(a)Define *n*-Scale

1. An n-scale is what we get when we split an octave into n sections. An n-scale has the following object designations: 0, 1,..., n − 1.

2. When listening to twelve-tone music, two tones that are 12 semitones apart are typically recognized. For this reason, the cyclic group (Zn, +) of order n is what we designate as an n-scale.Here, a scale is a sequence of notes or tones. Additionally, an octave is the standard way to span a scale with 12 notes, each spaced one semitone apart, such that the pitch before 0 is designated 11 and the pitch after 11 is named 0.

(b) Define transposing and inversion operation

1. Let us define *T* the operation of transposing as a permutation *T*:*Zn* → *Zn*, *a* |→ *T*(*a*): = 1+*a*. The group <*T*> is the cyclic group *ζn^*(*E*).

2. The operation of inversion can be defined as follows:a |→ I(a): = −a, Zn → Zn. The dihedral group ϑn ^(E) is the group <T, I>.

(c) Explain k-chord.

Assume that k <= n. In an n-scale, a subset of k Zn elements is called a k-chord.

2. Let G either equal ϑn ^(E) or ζn^(E). When two k-chords, A1 and A2, are equal, it means that there exists γ in G such that A2 = γ(A1).

(d) Example:

Let's take a closer look at traids, a subset of tones consisting of three different tones. Stated otherwise, we shall concentrate on the 3-chord, which is a subset of 3 Zn elements and represents a 12-scale.

We wish to apply Polya's Enumeration Theorem in this case:

Step 1: Define the cycle index of the group *G*, the cycle group of order 12 for example, and construct cycle index polynomial:

$$P_{C_{12}}(x_1,\ldots,x_{12}) = \frac{x_1^{12}}{12} + \frac{x_2^6}{12} + \frac{x_3^4}{6} + \frac{x_4^3}{6} + \frac{x_6^2}{6} + \frac{x_{12}}{3}.$$

Step 2: Determine colourings, black and white (same as including the note or not) and substitute expression of

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variable x, *x_i=b^i+w^i* for all *i:*

$$P_{C_{12}}(1+b,1+b^2,\ldots,1+b^{12}) = b^{12}+b^{11}+6b^{10}+19b^9+43b^8+66b^7+80b^6+66b^5+43b^4+19b^3+6b^2+b+1.$$

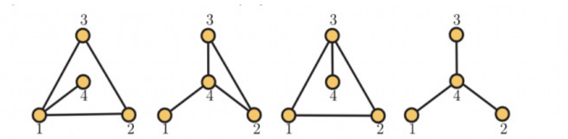
Step 3: Thus, we can deduce that the number of scales with k notes is the coefficient on *b^k*.

(3)Application in simple graph

(a) Counting the simple graphs with n vertex:

Each edge has the potential to be included or excluded, for a total of □(n,2). Consequently, on n vertices, there are $2^{C(n,2)}$ simple graphs.

As an illustration, we display four distinct labeled graphs on four vertices. However, the first three graphs displayed there are isomorphic to one another. Therefore, the image only shows two non-isomorphic graphs on four vertices.



(b) Example: Counting Non-Isomorphic Graphs for n=4

To illustrate the process, let's consider the case where n=4. Here, we need to count the number of non-isomorphic graphs with four vertices.

Step 1: Identifying Permutations

We begin by analyzing the symmetric group S_4, which represents all permutations of four vertices. To count non-isomorphic graphs, we consider the pair group S_4^2, which permutes the 2-element subsets of the set {1,2,3,4}. For simplicity, we denote a 2-element subset {i, j} by e_{ij}.

Step 2: Corresponding Permutations in Pair Group

For each permutation in S_4, we identify the corresponding permutation in S_4^2. For example, the identity permutation (1)(2)(3)(4) in S_4 corresponds to $(e_{12})(e_{13})(e_{14})(e_{23})(e_{24})(e_{34})$ in S_4^2. Similarly, other permutations such as (12)(3)(4) and (123)(4) correspond to distinct cycle structures in the pair group.

Step 3: Counting the Permutations

Next, we determine the number of permutations with each possible cycle structure in S_4^2. For instance, a permutation in S_4 with a single 4-cycle corresponds to a 4-cycle and a 2-cycle in S_4^2. The number of such permutations is given by 3!=6. Similarly, permutations with different cycle structures are counted, resulting in a detailed enumeration of all possible configurations.

combination	Number of possible order	Permutation in S_4.	Corresponding permutation in $S_4^{(2)}$
a single 4-cycle	6	(1,2,3,4)	$(e_{12}e_{23}e_{34}e_{14})(e_{24}e_{13})$
a 1- cycle and a 3-cycle	8	(1)(2,3,4)	$(e_{12}e_{13}e_{14})(e_{23}e_{34}e_{24})$
two 1-cycles and a 2-cycle	6	(1)(2)(3,4)	$(e_{12})(e_{13}e_{14})(e_{23}e_{24})(e_{34})$
two 2-cycles	3	(1,2)(3,4)	$(e_{12})(e_{13}e_{24})(e_{23}e_{14})(e_{34})$
Identity	1	(1)(2)(3)(4)	$(e_{12})(e_{13})(e_{14})(e_{23})(e_{24})(e_{34})$

Step 4: Cycle Structure and Generating Function

With the cycle structures identified, we can write the cycle index for the pair

group S_4^2 as:

$$P_{S_4^2}(x_1,\ldots,x_6)=\frac{1}{24}\left(x_1^6+9x_1^2x_2^2+8x_3^2+6x_2x_4\right)$$

To enumerate the graphs, we substitute $x_i=1+x$ for $1\leqslant i\leqslant 6$, which accounts for the presence or absence of each edge. This yields the generating function:

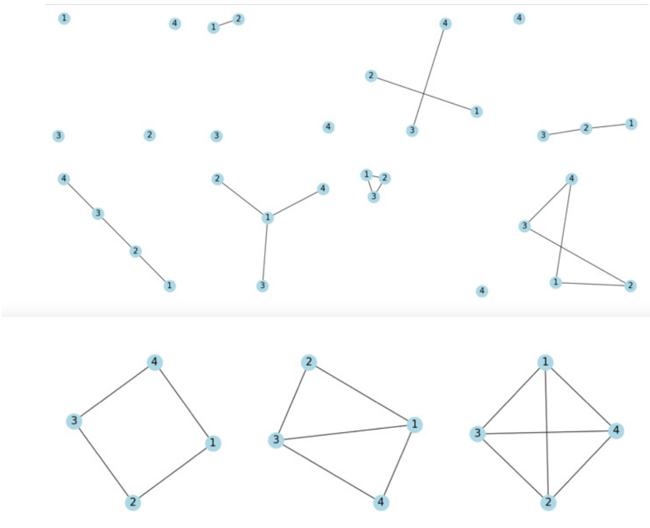
$$P_{S_4^2}(1+x,\ldots,1+x)=1+x+2x^2+3x^3+2x^4+x^5+x^6$$

This function indicates the number of 4-vertex graphs with m edges, where $0\leqslant m\leqslant 6$.

The number of non-isomorphic graphs with n vertex and k edges is given by the coefficient of x^i in the generating function.

(c) Conclusion:

By substituting x=1 into the generating function, on four vertices, we find that there exist eleven non-isomorphic graphs. This significant decrease from the 64 simple graphs emphasizes how crucial it is to take graph isomorphism into account while comparing distinct graph architectures. The method presented here provides a systematic approach to solving this problem, with potential applications in analyzing larger graphs or different graph types.



4. Conclusions

Based on the following, we can conclude that:

1) The number of specific isomers can be counted using Polya's enumeration theorem.

2)Polya's enumeration theorem can enumerate the number of chords with k notes in a typical 12-note scale.

3)Polya's enumeration theorem can count non-isomorphic graphs with n vertices.

Overall, Polya's theorem streamlines complex counting tasks by leveraging symmetry and rotation, making it a valuable tool in these diverse areas.

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