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Generalization of de Bruijn's extension of Pólya's theorem to all characters

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We generalize the de Bruijn extension of Pólya's theorem to all characters of finite permutation groups and show that the de Bruijn theorem becomes a special case of our generalization when applied to the character of the totally symmetric representation.

1. Introduction

In recent years the cross-fertilization of combinatorics and chemistry has led to numerous exciting developments and applications [1–16]. Applications of combinatorics to chemical problems range from a simple enumeration of isomers to more complex applications involving nuclear spin functions and character theory of finite groups. The intimate connection between combinatorics and character theory of finite groups dates back to the work of Frobenius, Littlewood, Foulks among others [17–20].

In 1937 Pólya [16] published a landmark paper which made significant impact both in mathematical and chemical literature, among other fields including computer science, finite automata and Boolean algebra. It is evident that the celebrated Pólya's theorem derived its motivation from the problem of enumerating isomers of organic compounds.

Following Pólya's theorem there were several authors who have expounded numerous ramifications and extensions. One such extension, originally due to de Bruijn [3], considers the case of two groups, one acting on the set of objects to be colored and the other group acting on two colors. Further generalization of this to a multi-colored problem (as opposed to the bi-colored problem) and the group acting on colors being any general group leads to the Harary–Palmer [14] power group enumeration theorem. While Pólya's theorem has received significant atten-

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tion in the chemical literature, chemical applications of de Bruijn's theorem or the Harary–Palmer power group theorem are little explored.

The present author [10,21] has considered extension of Pólya's theorem to other characters and their applications motivated by the works of Williamson [22], Merris [23], Foulks [20,24] and others. Of course, for the case of the symmetric groups (S_n) this extension simply leads to the famous Schur functions which are discussed in depth in several books [1,17–19]. To the best of the author's knowledge, the extension of de Bruijn's theorem to other characters is yet to be considered both in chemical and mathematical literature. Yet such an extension and further ramifications to the Harary–Palmer power group theorem could result in significant new applications to spectroscopy such as NMR, multiple-quantum NMR and ESR. The objective of this article is to consider a new generalization of de Bruijn's theorem to other characters. Section 2 considers the motivations and background information. Section 3 consists of the statement of the new theorem and illustrations.

2. Preliminaries

In ordinary Pólya's theorem, one considers D as a set of objects and R as a set of colors. Let G be a permutation group acting on D. Two maps f_1 and f_2 from D to R are said to be equivalent if there exists a $g \in G$ such that

$$f_1(d) = f_2(gd) \forall d \in D .$$

For each $r \in R$ assign a weight $w(r)$ and define the weight $W(f)$, the weight of a function $f : D \to R$ as

$$W(f) = \prod_{d \in D} w(f(d)) .$$

Define the cycle index P_G of the group G as

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

where $x_1^{b_1} x_2^{b_2} \dots x_n^{b_n}$ is a cycle representation for $g \in G$ if it generates b_1 cycles of length 1, b_2 cycles of length 2, etc., upon its action on the elements of the set D. Pólya's theorem yields a generating function for the equivalence classes of maps from $f : D \to R$ as follows:

$$\mathrm{GF} = P_G\left(x_k \to \sum_{r \in R} [w(r)]^k \right) ,$$

where the arrow symbol means replace every x_k in P_G by $\sum_{r \in R} [w(r)]^k$. This is also sometimes referred to as the Pólya substitution. The coefficient of a typical term $w_1^{b_1} w_2^{b_2} \dots w_n^{b_n}$ in the GF obtained thus yields the number of non-equivalent ways of coloring the vertices in the set D with b_1 colors of the first type (say white), b_2 colors of the second type (say yellow)..., b_n colors of the nth type (say green).

Consider an important modification to the ordinary cycle index P_G of the group G. Multiply the character $\chi(g)$ with each cycle representation. Then we will have a different cycle index for each irreducible representation Γ with character χ in the group G. This extension was called the generalized character cycle index (GCCI) by the current author [10,21]. In symbols it is defined as follows:

$$P_G^{\chi} = \frac{1}{|G|}\sum_{g\in G} \chi(g) x_1^{b_1} x_2^{b_2} \ldots x_n^{b_n},$$

where $\chi : g \to \chi(g)$ is the character of the irreducible representation Γ. The Pólya-like substitution in P_G^{χ} yields a generating function for each irreducible representation Γ. That is

$$\mathrm{GF}^{\chi} = P_G^{\chi}\left(x_k \to \sum_{r\in R} [w(r)]^k\right).$$

The interpretation of GF^{χ} for characters of irreducible representations other than A_1 (the totally symmetric representations) was given by the current author [21] for the first time. All functions $f : D \to R$ with the same weight W transform as a reducible representation in the group G. *The number of times an irreducible representation Γ occurs in this reducible representation is given by the coefficient of W in GF^{χ}.* Suppose W is of the form $w_1^{b_1} w_2^{b_2} \ldots w_n^{b_n}$, where $w_1, w_2, \ldots, w_n$ are the weights of different types of elements in the set R. Then the coefficient of $w_1^{b_1} w_2^{b_2} \ldots w_n^{b_n}$ gives the number of times the irreducible representation Γ occurs in the set of maps $f : D \to R$ such that all maps in the set have b_1 elements of the first kind, b_2 of the second kind, etc.

This generalization of Pólya's theorem to other characters was shown by the author [21,10] to result in some very significant and important applications in the areas of spectroscopy, dynamic stereochemistry and quantum chemistry.

3. De Bruijn's theorem and its generalizations to other characters

Consider a set D of objects and a set R of two different colors (say green and blue). Let G be a permutation group acting on D and in addition let H be a permutation group consisting of two elements $\{(\mathcal{B})(\mathcal{G}), (\mathcal{B}\mathcal{G})\}$. Note that H is the permutation group of colors and hence acts on the set R of colors. The first element in H is the identity while the second element corresponds to exchange (transposition) of colors.

Now consider all maps $f : D \to R$. These maps constitute a set which is denoted as R^D. The main difference between the problems considered in section 2 and the present section is that an *additional group H* acts on colors themselves. In the physical science area, this is sometimes referred to as color symmetry. This is diagrammatically illustrated in fig. 1. Suppose for convenience we denote the transposition of colors h. Two functions f_1 and f_2 are G-equivalent (as in Pólya's theorem) if there exists a $g \in G$, such that

$$f_1(d) = f_2(gd) \forall d \in D .$$

Now two different equivalence classes (patterns) under the action of G become equivalent if there are two representatives in these patterns such that one is transformable into the other by the action of h. In mathematical terms consider for each $g \in D$, $f \in R^D$, the mapping $\gamma_g : R^D \to R^D$ defined by

$$\gamma_g(f) = hfg ,$$

γ_g permutes R^D and $h \in H$. The de Bruijn theorem gives the number of distinct patterns (equivalence classes) under the action of both G on D and the permutation h on R.

THEOREM (DE BRUIJN)

The generating function for the equivalence classes of patterns under the action of both G and H is

$$P_G(x_k \to \mu_k) ,$$

$$\mu_k = \sum_{r \in R} w(r)w(hr) \ldots w(h^{k-1}r) ,$$

$$h^k r = r .$$

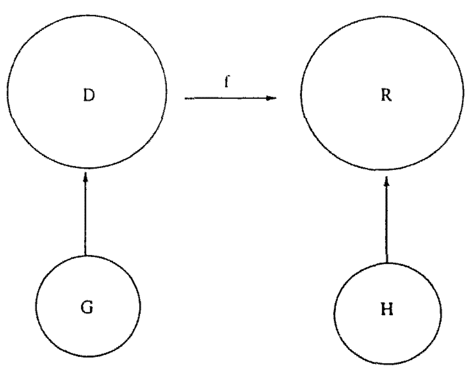

Fig. 1. Schematic illustration of map $f : D \to R$ and the action of G and H on the sets D and R, respectively. In the case of de Bruijn's theorem, the set R contains only two colors and the group H is composed of the identity permutation and the permutation of exchange of colors (elements of R).

Before we proceed to our generalization of de Bruijn's theorem to other characters, let us illustrate the theorem with an example first.

Consider the case of a tetrahedron. Let us color the vertices of the tetrahedron under the action of the T_d point group (G). Let R be a set of two colors say green and blue. The group H comprising two permutations is $H = [(\mathcal{G})(\mathcal{B}), (\mathcal{G}\mathcal{B})\}$. The cycle index of the T_d group for four vertices is

$$P_{T_d} = \frac{1}{24}[x_1^4 + 6x_1^2x_2 + 8x_1x_3 + 6x_4 + 3x_2^2].$$

In order to apply de Bruijn's theorem first, we need to construct μ_1, μ_2, etc. Since $h = (\mathcal{G}\mathcal{B})$ there is no h such that $hr = r$ for $r \in R$. Hence $\mu_1 = 0$. Since $h^2 = (\mathcal{G}\mathcal{B})(\mathcal{G}\mathcal{B}) = (\mathcal{G})(\mathcal{B})$ both green and blue colors in R are left invariant under the action of h^2. Hence

$$\mu_2 = \sum_{\mathcal{G},\mathcal{B}} w(r)w(hr) = 2\mathcal{G}\mathcal{B}.$$

It is seen that $\mu_3 = 0$ since $h^3 = h$. In general it can be shown that

$$\mu_k = \begin{cases} 2(\mathcal{G}\mathcal{B})^{k/2} & \text{if } k \text{ is even,} \\ 0 & \text{if } k \text{ is odd.} \end{cases}$$

Consequently, the equivalence classes under the action of both G and H is given by

$$P_G(x_k \to \mu_k)$$

or

$$\mathrm{GF} = \frac{1}{24}[0^4 + 6.0^2 + 8.0 + 6(2\mathcal{G}^2\mathcal{B}^2) + 3(2\mathcal{G}\mathcal{B})^2] = \mathcal{G}^2\mathcal{B}^2.$$

This means there is only one pattern which contains two green colors and two blue colors such that it remains invariant under the action of both G and H groups.

As yet another example, we consider the coloring of faces of the cube illustrated by Krishnamurthy [1]. The cycle index for the rotational subgroup O is given by

$$P_O = \frac{1}{24}[x_1^6 + 2x_1^2x_4 + 3x_1^2x_2^2 + 8x_3^2 + 6x_2^3].$$

For this case replacing every x_k by μ_k yields

$$\frac{1}{24}[6(2\mathcal{G}\mathcal{B})^3] = 2\mathcal{G}^3\mathcal{B}^3.$$

The two patterns are shown in fig. 2.

We now consider the generalization of de Bruijn's theorem to other characters. Consider the GCCI of the group G corresponding to the irreducible representation

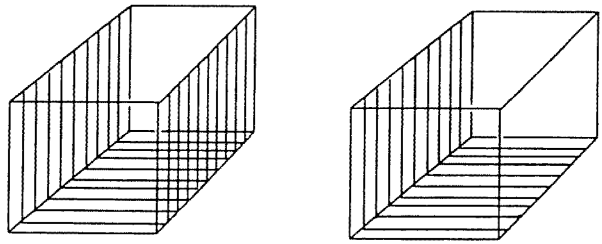

Fig. 2. Invariant patterns for coloring the faces of a cube under the action of both G and H.

Γ with character $\chi : g \rightarrow \chi(g)$ denoted by P_G^χ. We have already defined this in section 2. Let R be a set of two colors (say green and blue). Let H be the group of permutation of colors composed of $H = \{(\mathcal{G})(\mathcal{B}), (\mathcal{G}\mathcal{B})\}$. Let us also denote the permutation $(\mathcal{G}\mathcal{B})$ by h.

THEOREM

The GF_h^χ obtained by the following substitution yields the generating function for the transformation of maps $f : D \rightarrow R$ under the irreducible representation Γ,

$$\mathrm{GF}_h^\chi = P_G^\chi(x_k \rightarrow \mu_k) .$$

In the above substitution μ_k is obtained the same way as in the ordinary de Bruijn's theorem.

Let us illustrate this important extension of de Bruijn's theorem to other characters with an example. Consider the same problem of coloring the vertices of a tetrahedron with two different colors say green and blue $(\mathcal{G}, \mathcal{B})$. The T_d point group is also isomorphic to the S_4 group comprising 24 permutations of four objects. The relevant cycle indices of the five irreducible representations of the $T_d(S_4)$ group are shown below, where we use the standard $[P(n)]$, notation to denote the irreducible representations of S_4, $P(n)$ being the partition of an integer n,

$$P^{A_1} = P^{[4]} = \tfrac{1}{24}[x_1^4 + 6x_1^2x_2 + 8x_3 + 6x_4 + 3x_2^2] ,$$

$$P^{T_1} = P^{[31]} = \tfrac{1}{24}[3x_1^4 + 6x_1^2x_2 - 6x_4 - 3x_2^2] ,$$

$$P^{E} = P^{[2^2]} = \tfrac{1}{24}[2x_1^4 - 8x_1x_3 + 6x_2^2] ,$$

$$P^{T_2} = P^{[21^2]} = \tfrac{1}{24}[3x_1^4 - 6x_1^2x_2 + 6x_4 - 3x_2^2] ,$$

$$P^{A_2} = P^{[1^4]} = \tfrac{1}{24}[x_1^4 - 6x_1^2x_2 + 8x_1x_3 - 6x_4 + 3x_2^2] .$$

The μ_k quantities are defined the same way as in de Bruijn's theorem for this problem since we consider only the totally symmetric representation of the H group consisting of two permutations. Application of our theorem to the A_1 representation ($x_k \to \mu_k$) yields

$$\mathrm{GF}_h^{A_1} = \mathcal{G}^2\mathcal{B}^2 .$$

Note that this is identical to de Bruijn's theorem. Hence our theorem becomes de Bruijn's theorem for the totally symmetric A_1 representation. Let us now apply this to the T_1 representation

$$\mathrm{GF}_h^{T_1} = \tfrac{1}{24}[3 \cdot 0^4 + 6 \cdot 0^2 \cdot (2\mathcal{G}\mathcal{B}) - 6(2\mathcal{G}^2\mathcal{B}^2) - 3(2\mathcal{G}\mathcal{B})^2] = -\mathcal{G}^2\mathcal{B}^2 .$$

The $\mathrm{GF}_h^{A_1}$ suggests that there is one A_1 representation which contains two greens and two blues such that it remains invariant under the switching of blue to green and green to blue. The $\mathrm{GF}_h^{T_1}$, on the other hand, suggests the same thing but in addition due to the negative sign, the symmetry adapted combination of functions which contain two greens and two blues that transforms as the T_1 representation changes sign under the exchange of colors (blue $\to$ green and green $\to$ blue). Let us consider GF_h^{E}

$$\mathrm{GF}_h^{E} = \mathrm{GF}_h^{[2^2]} = \tfrac{1}{24}[2 \cdot 0^4 - 8 \cdot 0 \cdot 0 + 6(2\mathcal{G}\mathcal{B})^2] = \mathcal{G}^2\mathcal{B}^2 ,$$

$$\mathrm{GF}_h^{T_2} = \tfrac{1}{24}[3 \cdot 0^4 - 6 \cdot 0^2 \cdot (2\mathcal{G}\mathcal{B}) + 6(2\mathcal{G}^2\mathcal{B}^2) - 3(2\mathcal{G}\mathcal{B})^2] = 0 ,$$

$$\mathrm{GF}_h^{A_2} = \tfrac{1}{24}[0^4 - 6 \cdot 0^2 \cdot (2\mathcal{G}\mathcal{B}) + 8(0)(0) - 6(2\mathcal{G}^2\mathcal{B}^2) + 3(2\mathcal{G}\mathcal{B})^2] = 0 .$$

The above generating functions evidently suggest that among all functions which transform as the E representation only that which contains two greens and two blues is invariant to interchange of colors. Note that none of the functions in R^D which transform as T_2 and A_2 representations is invariant to interchange of colors as implied by $\mathrm{GF}_h^{T_2}$ and $\mathrm{GF}_h^{A_2}$.

4. Conclusion

Here we considered a generalization of de Bruijn's theorem to all characters of any finite permutation group. A physical interpretation for the generalization was also given. This important generalization can lead to several more powerful theorems. For example, the generalization of the Harary–Palmer power group enumeration theorem to other characters is a very important development. Likewise, one could consider other irreducible representations of the group H as well. It is not clear to the author at this time what this generalization of the Harary–Palmer power group theorem to the other characters of the group H would lead to in terms of physical applications. It is, however, evident that the present extension of de Bruijn's theorem to other irreducible representations will have important applications to NMR, ESR and multiple-quantum NMR spectroscopies. Such applications will be the topic of future studies.

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