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322. THE GENERATING FUNCTION FOR VARIATIONS WITH RESTRICTIONS AND PATHS OF THE GRAPH AND SELF-COMPLEMENTARY GRAPHS *

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In this paper the generating function for the numbers of variations with repetitions and a certain type of restrictions is determined. The variations in question are connected with paths in correspondent graph, so that the generating function for the numbers of paths in a graph is also given. Theorem 2. gives this function for complementary graph and for the sum and product of graphs. Finally, a spectral characteristic of self-complementary graph is given.

1. Variations with restrictions

Variation of the k-th class (also called: permutations k at a time) with repetitions of the set $X=\{x_1, \ldots, x_n\}$ is every ordered k-tuple $(x_{i_1}, \ldots, x_{i_k})$ where it need not be $x_{i_j} \neq x_{i_l}$. The number of such variations is $\overline{V}_n^k = n^k$.

During the formation of variations with repetitions it is possible to impose certain restrictions. In this article we shall consider variations with restrictions of the following type. For every $x_i \in X$, set X is decomposed into two disjoint sets X_{i1} and X_{i2}. In permitted variations there can appear after element x_i, which is not the last in that variation, only an element from the set X_{i1}. The first element is subjected to no restrictions.

A pair x_i, x_j of adjacent elements of a variation is called a *permitted pair* if and only if $x_j \in X_{i1}$. The square matrix $A = \| a_{ij} \|_1^n$, where $a_{ij}=1$ if x_i, x_j is a permitted pair and $a_{ij}=0$ otherwise, is caled the *matrix of permitted pairs*. $\overline{A}$ will denote the matrix obtained from A by interchanging 0 and 1. $\overline{A}$ is the *matrix of restrictions*.

We shall determine the number $\overline{V}_n^k(A)$ of variations with repetitions of k-th class of a set with n elements, with a given matrix of permitted pairs.

If A is interpreted as the adjacency matrix of graph G with vertices $x_1, \ldots, x_n$, it can easily be seen that the number $\overline{V}_n^k(A)$ is equal to the number of all paths of length $k-1$ in G. (Under „path of length k" we understand a sequence $u_1, \ldots, u_k$ of the lines of the graph, where it is not necessary that $u_i \neq u_j$ and where for $i=2, 3, \ldots, k$ the line u_i starts from that vertex in which

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u_{i-1} terminates. A line can be a loop. In case of undirected graphs every edge is to be replaced with two lines with mutually opposed orientations.)

It is known that the number of patsh of length k is determined by the use of the matix A^k. Namely, the element from the i-th row and j-th column of this matrix is equal to the number of paths of length k, which lead from the vertex x_i to the vertex x_j (see, for example, [1], p. 143).

If $\{Y\}$ denotes the sum of all elements of the matrix Y then

$$\overline{V}_n^k (A) = \{A^{k-1}\} \qquad (k=1, 2, \dots). \tag{1}$$

This, at least in principle, solves the question of the number of variations. However, when the order of A is high, expression (1) is unsuitable for practical calculations. We shall, therefore, starting from (1), deduce expressions which are more suitable in applications.

It is possible to deduce an explicit expression for $\overline{V}_n^k(A)$.

Let $\varphi(\lambda) = b_0 \lambda^m + b_1 \lambda^{m-1} + \cdots + b_m$ be minimal polynomial of A. Then

$$b_0 A^{m+k} + \cdots + b_m A^k = 0. \tag{2}$$

Introducing the notation $N_i = \{A^i\}$, (2) yields

$$b_0 N_{m+k} + \cdots + b_m N_k = 0. \tag{3}$$

Let $\lambda_1, \dots, \lambda_m$ be the zeros of the minimal polynomial $\varphi(\lambda)$. If we consider undirected graphs (A is, in that case, a symmetric matrix) these zeros are real and simple (see, for example, [2], p. 222). The solution of the difference equation (3) is, in that case, of the form

$$N_k = C_1 \lambda_1{}^k + \cdots + C_m \lambda_m{}^k = \overline{V}_n^{k+1}(A). \tag{4}$$

Constants $C_1, \dots, C_m$ can be determined if m quantities $N_0 = n$, $N_1, \dots,$ N_{m-1} are known.

As can be seen, lengthy calculations are here also necessary. Formula (4) is not useful if we are determining N_k for $k<m$. Besides, quantities C_i and λ_i are often irrational numbers (N_k is, of course, a natuaral number), which can imply numerical difficulties.

In connection with (4) we give a definition of *the main part of the spectrum* of the graph. The set of all the eigenvalues of adjacency matrix is called the spectrum of graph.

For the undirected graphs we define the main part of the spectrum of the graph. *The main part of the spectrum* contains all the eigenvalues λ_i $(i = 1, \dots, m)$ of the matrix A, which appear in the expression (4) and for which $C_i \neq 0$. In the main part of the spectrum all the eigenvalues are mutually distinct.

The other way of transforming the expression (1) uses the following formula from complex analysis (see, for example, [3], p. 119.)

$$f(A) = -\frac{1}{2\pi i} \oint_C f(z) (A - zI)^{-1} dz. \tag{5}$$

This formula holds if the function $f(z)$ and necessary number of its derivatives are defined on the spectrum of matrix A, where C is a simple contour containing the mentioned spectrum, and I is the unit matrix.

According to (1) and (5) we have

$$\overline{V}_n^k(A) = -\frac{1}{2\pi i}\oint_C z^{k-1}\{(A-zI)^{-1}\}\,dz. \tag{6}$$

Let $P_Y(\lambda)$ be the characteristic polynomial of matrix Y, i.e., $P_Y(\lambda) = \det(Y-\lambda I)$.

The following formula holds (see, for example, [4], p. 84):

$$\det(Y+tJ) = \det Y + t\{\mathrm{adj}\ Y\} \tag{7}$$

where t is a scalar and J is a square matrix whose elements are 1.

From (7), for $Y = A - zI$ and $t = -1$, we get

$$\begin{aligned}\{\mathrm{adj}\,(A-zI)\} &= \det(A-zI) - \det(A-zI-J) = \det(A-zI)\\ &-(-1)^n \det(J-A+zI) = \det(A-zI) - (-1)^n \det(\overline{A}+zI)\\ &= P_A(z) - (-1)^n P_{\overline{A}}(-z).\end{aligned} \tag{8}$$

According to (6) and (8) we have

$$\overline{V}_n^k(A) = -\frac{1}{2\pi i}\oint_C \frac{z^{k-1}}{P_A(z)}\{\mathrm{adj}\,(A-zI)\}\,dz = -\frac{1}{2\pi i}\oint_C z^{k-1}\frac{P_A(z)-(-1)^n P_{\overline{A}}(-z)}{P_A(z)}\,dz,$$

i. e.,

$$\overline{V}_n^k(A) = \frac{(-1)^n}{2\pi i}\oint_C z^{k-1}\frac{P_{\overline{A}}(-z)}{P_A(z)}\,dz, \quad (k=1,2,\ldots). \tag{9}$$

Calculation of integral (9) by the theorem of residues again yields relation (4). In this way we obtain at the same time coefficients C_i from (4).

However, it is possible to avoid calculating an integer by the use of irrational numbers.

The function $\frac{P_A(-z)}{P_{\overline{A}}(z)} = R(z)$ can be developed in the vicinity of $z = \infty$ into a series of the form $R(z) = \sum_{i=0}^{+\infty} \frac{B_i}{z^i}$. This expression holds outside every circle $|z| = r$, which contains the spectrum of matrix A. (9) now becomes

$$\overline{V}_n^k(A) = \frac{(-1)^n}{2\pi i}\oint_C \left(\sum_{i=0}^{+\infty}\frac{B_i}{z^{i-k+1}}\right)dz = (-1)^n B_k. \tag{10}$$

This actually proves the following

Theorem 1. *The function*

$$G(t) = (-1)^n \frac{P_{\overline{A}}\left(-\frac{1}{t}\right)}{P_A\left(\frac{1}{t}\right)} \tag{11}$$

is generating function for the numbers $\overline{V}_n^k$ (A) *of the variations of k-th class with repetitions and with the matrix of permitted pairs A, where the following relation holds*

$$(12) \qquad \overline{V}_n^k(A)=\frac{1}{k!}G^{(k)}(0) \qquad (k=1,2,\ldots).$$

For $k=0$ *one obtains* $\overline{V}_n^0(A)=1$.

The MACLAURIN series of a rational function can be obtained by dividing the polynomial in numerator by the polynomial in denominator, where one always divides the lowest powers of these polynomials. Since the coefficients of the mentioned polynomials are integers, the process of calculating the number of variations does not lead outside the set of integers. In certain cases calculating by use of the generating function is more economic than the direct application of formula (1).

2. Paths in the graph

From (1) and (12) it follows, that the generating function $H_G(t)=\sum_{k=0}^{+\infty} N_k t^k$ for the numbers N_k of the paths of the lengths k, of the graph G, with the adjacency matrix A, is given by the expression

$$(13) \qquad H_G(t)=\frac{1}{t}\left[(-1)^n\frac{P_{\overline{A}}\left(-\frac{1}{t}\right)}{P_A\left(\frac{1}{t}\right)}-1\right].$$

This expression holds in the most general case, i.e.. G can have loops and multiple edges. In the further text we shall understand, that G is an undirected graph without loops and multiple edges. $\overline{G}$ denotes the graph complementary to the graph G, and G' the graph, which can be obtained, if to each of the vertices of G one loop is added. The adjacency matrix of the graph $\overline{G}$ is $\overline{A}$-I, and of G' is $A+I$.

We consider also the following type of sum and product of two undirected graphs G_1 and G_2, without loops and multiple edges.

The graph G_1+G_2 contains all the vertices and all the edges of the graphs G_1 and G_2, and only them.

The graph $G_1\times G_2$ one obtains from the graph G_1+G_2, if each of the vertices of G_1 is joined by one edge with each of the vertices of G_2.

This sum and product were considered in [5]. According to this paper, a graph is called elementary if it is connected and cannot be represented as the product of two disjoint graphs, Clearly,

$$(14) \qquad \overline{G_1\times G_2}=\overline{G}_1+\overline{G}_2.$$

From the obvious relation

(15) $$P_{X+I}(\lambda)=P_X(\lambda-1)$$

and from (13) one obtains the following form of the generating function:

(16) $$H_G(t)=\frac{1}{t}\left[(-1)^n\frac{P_{\bar{G}}\left(-\frac{t+1}{t}\right)}{P_G\left(\frac{1}{t}\right)}-1\right].$$

Theorem 2. *For the generating function $H_G(t)$ for the numbers of paths of the graph G the following formulas hold:*

(17) $$H_{G'}(t)=\frac{1}{1-t}H_G\left(\frac{t}{1-t}\right),$$

(18) $$H_{\bar{G}}(t)=\frac{H_G\left(-\frac{t}{t+1}\right)}{t+1-t\,H_G\left(-\frac{t}{t+1}\right)},$$

(19) $$H_{G_1+G_2}(t)=H_{G_1}(t)+H_{G_2}(t),$$

(20) $$H_{G_1\times G_2}(t)=\frac{H_{G_1}(t)+H_{G_2}(t)+2t\,H_{G_1}(t)\,H_{G_2}(t)}{1-t^2\,H_{G_1}(t)\,H_{G_2}(t)}.$$

Proof. According to (13) and (15) we have

$$H_{G'}(t)=\frac{1}{t}\left[(-1)^n\frac{P_{J-A-I}\left(-\frac{1}{t}\right)}{P_{A+I}\left(\frac{1}{t}\right)}-1\right]$$

$$=\frac{1}{t}\left[(-1)^n\frac{P_{J-A}\left(-\frac{1}{t}+1\right)}{P_A\left(\frac{1}{t}-1\right)}-1\right]$$

$$=\frac{1}{1-t}\;\frac{1}{\frac{t}{1-t}}\left[(-1)^n\frac{P_{J-A}\left(-\frac{1}{\frac{t}{1-t}}\right)}{P_A\left(\frac{1}{\frac{t}{1-t}}\right)}-1\right]=\frac{1}{1-t}H_G\left(\frac{t}{1-t}\right),$$

which proves (17).

(18) can be directly verified if one uses (16) and the folowing, its analogous, formula:

$$H_{\overline{G}}(t) = \frac{1}{t}\left[(-1)^n \frac{P_G\left(-\frac{t+1}{t}\right)}{P_{\overline{G}}\left(\frac{1}{t}\right)} - 1\right].$$

The relation (19) is obvious.

For the proof of the relation (20), one uses the relations (14), (18) and (19):

$$H_{G_1 \times G_2}(t) = H_{\overline{\overline{G}_1 + \overline{G}_2}} = \frac{H_{\overline{G}_1 + \overline{G}_2}\left(-\frac{t}{t+1}\right)}{t+1-t\, H_{\overline{G}_1 + \overline{G}_2}\left(-\frac{t}{t+1}\right)}$$

(21) $$= \frac{H_{\overline{G}_1}\left(-\frac{t}{t+1}\right) + H_{\overline{G}_2}\left(-\frac{t}{t+1}\right)}{t+1-t\left(H_{\overline{G}_1}\left(-\frac{t}{t+1}\right) + H_{\overline{G}_2}\left(-\frac{t}{t+1}\right)\right)}.$$

From (18) one obtains

(22) $$H_{\overline{G}}\left(-\frac{t}{t+1}\right) = \frac{(t+1)\, H_G(t)}{1 + t\, H_G(t)}.$$

Using (22) from (21) one obtains (20).

Examples. According to Theorem 2, the generating function for every graph can be obtained if we know the generating functions for the elementary graphs. A regular graph of the degree m, with n vertices, has, obviously $N_k = nm^k$ paths of the lengths k, and therefore

(23) $$H_G(t) = \sum_{k=0}^{+\infty} nm^k t^k = \frac{n}{1-mt}.$$

For $m = n-1$ one obtains the complete graphs and for $m = 0$ the graph, which contains only isolated vertices. The graph, which has only one vertex without edges and loops, has the generating fuction of the form $H_G(t) = 1$.

The bicomplete graph K_{n_1, n_2} can be represented as the product of graphs G_1 and G_2, both of which contain only isolated vertices. We then have $H_{G_1}(t) = n_1$ and $H_{G_2}(t) = n_2$, and according to (20), for the bicomplete graph we have

(24) $$H_{K_{n_1, n_2}}(t) = \frac{n_1 + n_2 + 2n_1 n_2 t}{1 - n_1 n_2 t^2}.$$

Specially, for $n_1 = n$ and $n_2 = 1$ the considered graph represents a star and corresponding generating function is

(25) $$H_{K_{n,1}}(t) = \frac{n+1+2nt}{1-nt^2}.$$

3. Self-complementary graphs

The graph G is called self-complementary, if it is isomorphic to its complementary graph G. Then we have $P_{\bar{G}}(t)=P_G(t)$ and the generating function of the numbers of paths reads

$$H_G(t)=\frac{1}{t}\left[(-1)^n\frac{P_G\left(-\frac{t+1}{t}\right)}{P_G\left(\frac{1}{t}\right)}-1\right]. \tag{26}$$

From this expression the spectral characteristic of the self-complementary graphs can be derived, given by the following theorem.

Theorem 3. *Let G be a self-complementary graph and λ_i an eigenvalue from its spetcrum, of the multiplicity $p_i(>1)$, (if it exists). Then to eigenvalue λ_i corresponds another eigenvalue λ_j, whose multiplicity is not less than p_i-1, where $\lambda_i+\lambda_j=-1$.*

Proof. Let the spectrum of the graph G be formed by the eigenvalues $\lambda_1, \ldots, \lambda_n$. Putting $\frac{1}{t}=u$, we have

$$H_G(t)=u\left[\frac{(u+\lambda_1+1)\cdots(u+\lambda_n+1)}{(u-\lambda_1)\cdots(u-\lambda_n)}-1\right]. \tag{27}$$

According to the definition of the generating function and according to (4) we have

$$\psi(u)=\frac{(u+\lambda_1+1)\cdots(u+\lambda_n+1)}{(u-\lambda_1)\cdots(u-\lambda_n)}=1+\sum_{k=0}^{+\infty}\frac{N_k}{u^{k+1}}=1+\sum_{i=1}^{m}\frac{C_i}{u-\lambda_i}. \tag{28}$$

We see that $\psi(u)$ must be a rational function having only simple poles. The set of these poles is equal to the main part of the spectrum of the graph. Thus, multiple factors in expression (28) denominator have to be cancelled, so that, after all possible cancellations, the zeros of the polynomial in the denominator represent the main part of the spectrum.

The statement of Theorem 3 follows from this fact.

Remark. In [6] an analogous theorem for the regular self-complementary graphs is proved. That theorem can be proved analogously to Theorem 3 from this paper, if one has in mind, that the main part of the spectrum of a regular graph contains only the greatest number from the spectrum.

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