Distance Polynomial and Characterization of a Graph

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Introduction

A graph G with N points is equivalent to an adjacency matrix $\boldsymbol{A}$ of the order N with elements,

$$(A)_{ij}=\begin{cases} 1 & \text{if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

However, the number of the bits of information necessary for the characterization of a graph increases with the square of N, causing a serious problem for larger graphs. Many attempts have been done to get such a characteristic quantity or index that uniquely corresponds to a given graph. It has been shown that neither of the characteristic polynomial[1-3]

$$P(X)=(-1)^N \det|\boldsymbol{A}-X\boldsymbol{E}| \tag{2}$$

nor the topological index Z[4-6] uniquely determines the topology of a graph, although a number of interesting relations have been discovered.[7-10]

In this paper we give a preliminary account of the interesting properties of a newly proposed quantity, a distance polynomial, and present a conjecture that it might be used as the characterization of a graph.

Definition

Since we are concerned only with non-directed graphs, a distance matrix $\boldsymbol{D}$ is an $N\times N$ symmetric matrix with elements,[11]

$$(D)_{ij}=\begin{cases} \text{the number of the lines of the} \\ \text{shortest path from } i \text{ to } j, \end{cases} \tag{3}$$

and a distance polynomial $S(X)$ is defined as

$$S(X) = (-1)^N \det|\boldsymbol{D} - X\boldsymbol{E}|$$

$$= \sum_{k=0}^{N} a_k X^{N-k}. \tag{4}$$

Tree Graphs

For a series of path progressions (linear chains without branches) $S(X)$'s are obtained as in Table I, from which we get the following relation.

Table I. Distance polynomials of linear chains.[a)]

G	N	C_k k=2	3	4	5	6
•	1					
—	2	1				
— —	3	6	4			
— — —	4	20	32	12		
— — — —	5	50	140	120	32	
— — — — —	6	105	448	648	384	80

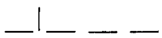
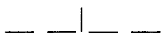
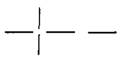
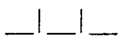
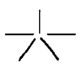
a) $S(X) = X^N - \sum_{k=2}^{N} C_k X^{N-k}$

THEOREM 1. *The distance polynomial of a path progression with N points is given by*

$$S(X) = X^N - \sum_{k=2}^{N} 2^{k-2}(k-1)\frac{N^2(N^2-1^2)(N^2-2^2)\cdots(N^2-\overline{k-1}^2)}{k^2(k^2-1^2)(k^2-2^2)\cdots(k^2-\overline{k-1}^2)} X^{N-k}. \tag{5}$$

Similarly for chain graphs with branches, $S(X)$'s are obtained as in Table II. From a large number of $S(X)$'s of tree graphs the following relations for the values of the expansion coefficients were proved by induction.

Table II. Distance polynomials of branched trees.[a)]

G	N	C_k k=2	3	4	5	6
	4	15	28	12		
	5	38	116	112	32	
	5	28	88	96	32	
	6	84	368	580	368	80
	6	77	356	572	368	80
	6	60	272	468	336	80
	6	65	296	504	352	80
	6	45	200	360	288	80

a) See the footnote of Table I.

THEOREM 2. *The coefficients of the X^N and X^{N-1} for a non-directed graph are respectively unity and zero.*

$$a_0=1 \tag{6}$$

$$a_1=0 \tag{7}$$

THEOREM 3. *The coefficient of the X^{N-2} term (neck) for a non-directed graph is the trigonal sum of the squares of the distance matrix,*

$$a_2=-\sum_{i>j}^{N}(D)^2_{ij}. \tag{8}$$

THEOREM 4. *All the tree graphs with N points have the same tail (the last term),*

$$a_N=-2^{N-2}(N-1). \qquad (tree) \tag{9}$$

THEOREM 5. *The coefficient of the X term (hip) of a tree graph is*

$$a_{N-1}=-2^{N-3}\sum_m n_m(m-1)(2N-m+2), \qquad (tree) \tag{10}$$

where n_m is the number of points with degree m, which is the number of the neighbors to a point.

Theorem 5 can be expressed symbolically as

$$a_{N-1} = -2^{N-3}[2N(\text{— —}) + 2(2N-1)(\text{\_|\_}) + 3(2N-2)(\text{—|—}) + 4(2N-3)(\text{—|—, with two lower branches}) + \cdots], \qquad \text{(tree)} \qquad (11)$$

where a pair of round brackets mean the number of points with degree 2, 3, 4, and so on.

Other expansion coefficients a_k's could be formulated but would inevitably be complicated.

Cycle Graphs without Branches

For a series of monocyclic graphs without branches $S(X)$'s are obtained as in Table III and we get

THEOREM 6. *The $S(X)$ of an N-membered cycle is given by*

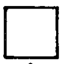
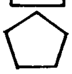
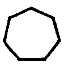
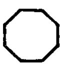
$$S(X) = X^{m-1}(X-m^2)[X^m + \sum_{k=1}^{m} 2^{2(k-1)} \frac{m}{k} \, {}_{m+k-1}C_{2k-1} X^{m-k}]$$

$$= X^{2m} - \sum_{k=2}^{m} 2^{2k-3}[m^2(2k^2-k-2)+2(k-1)^2] \times \frac{m^2(m^2-1^2)(m^2-2^2)\cdots(m^2-\overline{k-2}^2)X^{2m-k}}{k^2(k^2-1^2)(k^2-2^2)\cdots(k^2-\overline{k-2}^2)(k^2-\overline{k-1}^2)} - 2^{2(m-1)}m^2X^{m-1}$$

$$(N=2m) \qquad (12)$$

$$S(X) = [X-m(m+1)]\,[\sum_{k=0}^{m} {}_{m+k}C_{2k} X^{m-k}]^2. \qquad (N=2m+1) \qquad (13)$$

Table III. Distance polynomials of cycles.[a]

G	N	c_k k=2	3	4	5	6	7
	3	3	2				
	4	12	16				
	5	25	60	35	6		
	6	57	200	144			
	7	98	490	707	434	119	12
	8	176	1152	1984	1024		

a) See the footnote of Table I.

No simple expanded form of Eq. (13) was obtained. Theorems 2 and 3 are also valid for graphs with cycles.

COLLORARY. *The tail of an N-membered cycle is given by*

$$-2^{N-4}N^2X^{N/2-1} \qquad (N=2m) \tag{14}$$

$$-(N^2-1)/4. \qquad (N=2m+1). \tag{15}$$

Cycle Graphs with Branches

In Table IV $S(X)$'s of all the possible graphs with $N=5$ are shown. Note that the ring skeleton of the graphs Nos. 4–6 is a triangle and they all have the same tail -20. The graphs Nos. 11–13 have the same tail but the ring skeleton of the graph No. 13 is different from those of the others. In this respect we have examined the distance polynomials of more than five hundreds graphs and got the following conclusion.

THEOREM 7 (Conjecture). *The tail of the distance polynomial of a given graph is determined only by the number of points and the ring skeleton.*

As a special case for graphs containing one cycle we get

THEOREM 8. *The tail of a graph with N points and an M-membered cycle is*

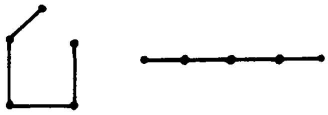
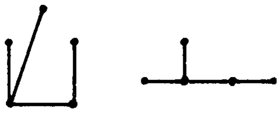
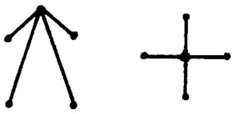
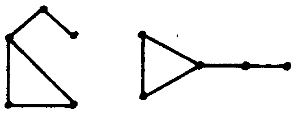
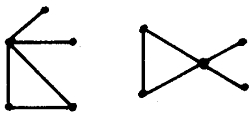
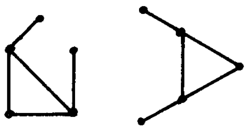
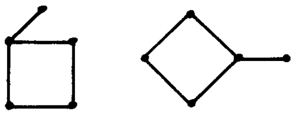
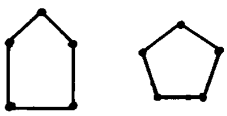
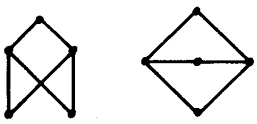
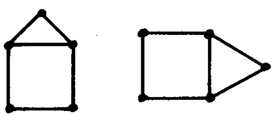
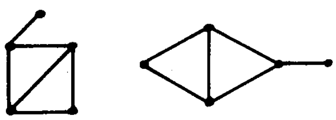
$$-2^{N-3}[MN-M^2/2]X^{M/2-1} \qquad (M=2m) \tag{16}$$

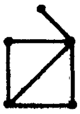
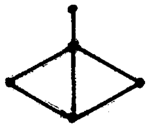
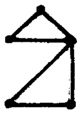
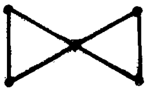
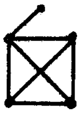
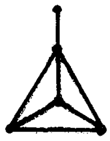
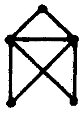
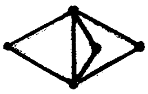
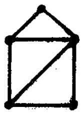
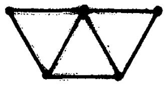
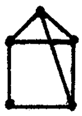
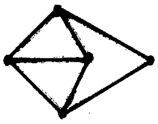
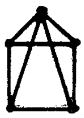
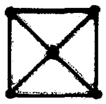
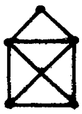
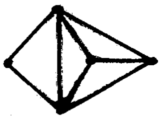
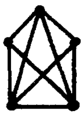
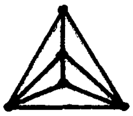
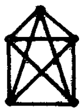
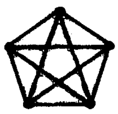
$$-2^{N-M-1}[MN-(M^2+1)/2]. \qquad (M=2m+1) \tag{17}$$

Note that Theorem 4 can be derived by the substitution of either $M=2$ into Eq. (16) or $M=1$ into Eq. (17).

Let us again see Table IV. The coefficients of a distance polynomial have full informations for the topology of the graph concerned. Namely, the head (X^N) gives the number of points, the neck (a_2X^{N-2}) reflects the roundness of the graph, the tail (a_tX^{N-t}) is dependent of the ring skeleton, and the hip ($a_{t-1}X^{N-t+1}$) is a function of the branching. Thus one may conjecture that the distance polynomial or its coefficients could be used for the characterization of a graph. Further study for graphs with more than one cycle is being in progress.

Table IV. Distance polynomials of graphs with $N=5$.[a)]

No.	G[b)]	C_k k=2	3	4	5
1		50	140	120	32
2		38	116	112	32
3		28	88	96	32
4		35	88	74	20
5		25	70	66	20
6		30	82	72	20
7		30	76	48	
8		25	60	35	6
9		22	52	24	−16
10		22	50	28	
11		27	64	50	12

12			22	56	46	12
13			22	52	43	12
14			19	44	36	10
15			19	46	36	8
16			19	42	29	6
17			19	40	18	–4
18			16	32	16	
19			16	34	25	6
20			13	26	18	4
21			10	20	15	4

a) See the footnote of Table I.
b) Two graphs in a row are isomorphic. The left graphs are taken from the Appendix of Ref. 11.

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