Aplikace matematiky

Pavel Křivka; Nenad Trinajstić On the distance polynomial of a graph

Aplikace matematiky, Vol. 28 (1983), No. 5, 357-363

Persistent URL: http://dml.cz/dmlcz/104047

Terms of use:

© Institute of Mathematics AS CR, 1983

Institute of Mathematics of the Czech Academy of Sciences provides access to digitized documents strictly for personal use. Each copy of any part of this document must contain these *Terms of use*.



This document has been digitized, optimized for electronic delivery and stamped with digital signature within the project *DML-GZ: The Czech Digital Mathematics Library* http://dml.cz

ON THE DISTANCE POLYNOMIAL OF A GRAPH

Pavel Křivka, Nenad Trinajstić (Received December 29, 1982)

The distance matrix, which is a structure less common than the adjacency matrix [1], has been increasingly used in recent years in several different areas such as anthropology [2], [3], graph theory [4]–[6], theory of communication [7], chemistry [8]-[10], history [11], etc.

The distance matrix (which is sometimes also called the metrics matrix) is, in a sense, a more complicated and also a richer structure than the adjacency matrix. While each (0, 1) symmetric matrix in which each diagonal entry is zero corresponds to a unique graph or digraph, this is not the case with the distance matrix (which is a symmetric matrix with diagonal entries zero, but not (0, 1)). We will consider finite connected graphs without loops. Graphs will be symbolized by G. The distance matrix \mathbf{D} has the entries $d_{ii} = 0$ and $d_{ij} =$ the length of the shortest path between the vertices i and j. The distance polynomial of G is defined as det $|x\mathbf{I} - \mathbf{D}|$ where \mathbf{I} is the unit matrix.

Proposition 1. Every root of the distance polynomial is real.

Proof. The eigenvalues of a symmetric matrix are always real [12].

Proposition 2. The coefficient a_{n-1} at x^{n-1} is always zero.

Proof. Follows from the development of the determinant.

Proposition 3. The distance polynomial of a complete graph with n vertices equals $(x + 1)^{n-1} (x - n + 1)$.

Proof. For complete graphs the distance matrix coincides with the adjacent matrix.

Proposition 4. The sum of the roots of the distance polynomial is zero.

Proof. The sum of roots is equal to the trace of D which is zero since G has no loops.

Proposition 5. The sum of the squares of the roots of the distance polynomial is equal to $\sum d_{ij}^2$ (the sum is through all pairs i, j and each pairs is taken twice -(i,j) and (j,i)).

Proof. The sum of the squares of the roots is equal to the trace of \mathbf{D}^2 .

Proposition 6. If there are two vertices with the same neighbourhood in G, then one root of the distance polynomial is either -1 (if the vertices are adjacent) or -2 (if the two vertices are not adjacent).

Proof. If the two vertices are adjacent, the distance between them is 1. If the two vertices are not adjacent, the distance between them is 2, otherwise the corresponding rows in \mathbf{D} are the same. After subtracting these two rows, we obtain before the determinant either (x + 1) or (x + 2).

Proposition 7. If G is a path on n+1 vertices $(n \ge 3)$, then $a_0 = (-1) n 2^{n-1}$, where a_0 is a constant coefficient, i.e. $a_0 = \det |-\mathbf{D}|$.

Proof. By directly calculating the determinant

(1)
$$\det |\mathbf{D}| = \begin{vmatrix} 0 & 1 & 2 & 3 & \dots & n \\ 1 & 0 & 1 & 2 & \dots & n-1 \\ 2 & 1 & 0 & 1 & \dots & n-2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ n & n-1 & \vdots & \dots & 0 \end{vmatrix}$$

First we subtract the *n*-th column from the (n + 1)-st and afterwards we add the last row to all the precedings ones, so that in the last column we obtain all zeros except the entry $a_{n+1,n+1} = -1$.

(2)
$$\begin{vmatrix} n & n & n & \dots & n & 0 \\ n+1 & n-1 & n-1 & \dots & n-1 & 0 \\ n+2 & n & n-2 & \dots & n-2 & 0 \\ \vdots & \vdots & & & & \vdots \\ 2n-1 & \vdots & \ddots & \ddots & 0 \\ n & \vdots & & \ddots & \ddots & 0 \\ n & \vdots & & \ddots & \ddots & 1 \end{vmatrix} =$$

$$= (-1) n \begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ n+1 & n-1 & n-1 & \dots & n-1 \\ n+2 & n & n-2 & \dots & n-2 \\ \vdots & \vdots & & \ddots & \vdots \\ 2n-1 & \vdots & \ddots & \ddots & 1 \end{vmatrix}$$

The resulting determinant can be expanded with respect to the last column and n put in front of the determinant. Next we subtract the last column from all the preceding ones and expand with respect to the first row:

(3)
$$(-1) n(-1)^{n+1} \begin{vmatrix} 2 & 0 & 0 & \dots & 0 \\ 4 & 2 & 0 & \dots & 0 \\ 6 & 4 & 2 & \dots & \dots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 2n-2 & 2n-4 & \dots & 2 \end{vmatrix} = (-1)_{n+2} n 2^{n-1}$$

Because det $|-\mathbf{D}| = (-1)^{n+1}$ det $|\mathbf{D}|$, we have $a_0 = (-1)^{2n+3} n 2^{n-1} = -n \cdot 2^{n-1}$, q.e.d.

Proposition 8. For complete bipartite graphs $K_{m,n}$, the roots are -2(m+n-2) times) and the remaining two roots are given by the following equations:

$$x_1^2 + x_2^2 = 2(2m^2 - 4m + 2n^2 - 4n + mn + 4)$$

 $x_1 + x_2 = 2(m + n - 2)$

Proof. We can write the distance polynomial of $K_{m,n}$ in the form

(4)
$$\det |x\mathbf{I} - \mathbf{D}| = \begin{vmatrix} x & \dots & -2 \\ \vdots & \ddots & \vdots \\ -2 & \dots & x \\ \hline \mathbf{B}^{\mathsf{T}} & \vdots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ -2 & \dots & x \end{vmatrix}$$

where **B** denotes the $(m \times n)$ matrix consisting entirely of -1's. By subtracting the second row the first, the third from the second, until m-th from the (m-1)-st, and the (m+2)-nd from the (m+1)-st, etc., we obtain the following determinant

We immediately see that m+n-2 eigenvalues are -2. According to Proposition 5, we have $\sum x_i^2 = \sum_{i,j} d_{ij}^2 = 4m(m-1) + 4n(n-1) + 2mn = 4m^2 - 4m + 4n^2 - 4m + 4mn$ and as $\sum_{i=3}^{m+n} x_i^2 = 4(m+n-2)$, we have $x_1^2 + x_2^2 = 2(2m^2 + 2n^2 - 4m - 4n + mn + 4)$. According to Proposition 4, we have $x_1 + x_2 - 2(m + n - 2) = 0$.

Proposition 9. If G is a star with n vertices, then

$$\det |x\mathbf{I} - \mathbf{D}| = (x+2)^{n-2} (x^2 - 1 - (n-2)(2x+1)).$$

The distance polynomial of the star graph will be denoted by S_n .

Proof. The distance polynomial of a star is given by

(6)
$$S_{n} = \begin{vmatrix} x & -1 & -1 & \dots & -1 \\ -1 & x & -2 & \dots & -2 \\ -1 & -2 & x & \dots & -2 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ -1 & -2 & -2 & \dots & x \end{vmatrix}$$

By subtracting the (n-1)-st row from the *n*-th row, we can put the factor (x+2) (from the last row) in front of the determinant and expand it with respect to the last row:

(7)
$$S_{n} = (x+2) \left(\begin{vmatrix} x-1 & -1 & \dots & -1 \\ -1 & x-2 & \dots & -2 \\ -1 & -2 & x & \dots & -2 \end{vmatrix} + \begin{vmatrix} x-1 & -1 & \dots & -1 \\ -1 & x-2 & \dots & -2 \\ -1 & -2 & x & \dots & -2 \end{vmatrix} \right)$$

The second determinant evidently corresponds to S_{n-1} . The first determinant differs from the second one only in the entry $d_{n-1,n-1} = -2$. If we denote this one by \overline{S}_{n-1} , we obtain the recurrent formula

(8)
$$S_n = (x+2)(\overline{S}_{n-1} + S_{n-1}).$$

Now, if we consider the determinant \overline{S}_n , we obtain by the same procedure the formula

$$\overline{S}_n = (x+2)\,\overline{S}_{n-1}\,.$$

Combining (8) and (9) we obtain

(10)
$$S_n = (x+2)^{n-2} \left(S_2 + (n-2) \, \overline{S}_2 \right)$$

and

$$S_2 = \begin{vmatrix} x & -1 \\ -1 & x \end{vmatrix} = x^2 - 1,$$

$$\overline{S}_2 = \begin{vmatrix} x & -1 \\ -1 & -2 \end{vmatrix} = -2x - 1, \quad \text{q.e.d.}$$

Proposition 10. If G is an even cycle, then at least one root of the distance polynomial is zero.

Proof. It suffices to prove that det |D| = 0.

By adding the first row to the (n/2 + 1)-st one and the second row to the (n/2 + 2)-nd one, we get two identical rows, namely the (n/2 + 1)-st and the (n/2 + 2)-nd, q.e.d.

Comment. Since the distance matrix for cycles is a circulant matrix, we can obtain its roots by means of rules for the corresponding determinant [13].

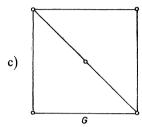
Examples.

a)
$$C_3$$
 – cycle

$$\det |xI - D| = (x - 2)(x + 1)^2$$

b)
$$C_{4}$$
-cycle

$$\det |xI - D| = (x + 2)^2 (x - 4) x$$



$$\det |xI - D| = (x + 2)^3 (x^2 - 6x + 2)$$

References

- [1] F. Harary: Graph theory. Addison-Wesley. Reading, Mass. 1971, pp. 150-152.
- [2] P. Hage: A graph theoretic approach to alliance structure and local grouping in highland New Quinea, Anthropol. Forum 3 (1973/74), 280—294.
- [3] P. Hage: Graph theory as a structural model in cultural anthropology, Ann. Rev. Anthropol. 8 (1979) 115-136.
- [4] M. Eldelberg, M. R. Garey, and R. L. Graham: On the distance matrix of a tree, Discrete Math. 14 (1976) 23-29.
- [5] R. L. Graham, A. J. Hoffman, and H. Hosoya: On the distance matrix of a directed graph, J. Graph Theory 1 (1977) 85-88.
- [6] A. J. Hoffman and M. H. McAndrew: The polynomial of a directed graph, Proc. Amer. Math. Society 16 (1965) 303.
- [7] R. L. Graham and H. O. Pollak: On the addressing problem for loop switching, Bell Sys. Tech. J. 50 (1971) 2495—2519.
- [8] D. H. Rouvray: The topological matrix in quantum chemistry, in: Chemical applications of graph theory, ed. by A. Balaban, Academic, London 1976, pp. 175-221.
- [9] D. Bonchev and N. Trinajstić: Information theory, distance matrix, and molecular branching,
 J. Chem. Phys. 67 (1977) 4517—4533.
- [10] N. Trinajstić: Chemical graph theory, CRC, Boca Raton, Florida, 1983.
- [11] G. Irwin: The emergence of a central place in coastal Papuan prehistory: A theoretical approach, Mankind 9 (1974) 268-272.
- [12] A. Kurosh: Higher algebra, Mir, Moscow 1980.
- [13] M. Marcus and H. Minc: A survey of matrix theory and matrix inequalities, Allyn and Bacon, Boston 1964.

Note added in proof. Proposition 7 holds generally for any tree as was first proved in [7]. By an accident we overlooked a paper [a] which contains without proofs

some theorems related to our work. Some other related references can be found in the second edition of the book [b] that came only recently into our hands.

- [a] H. Hosoya, M. Murakami and M. Gotoh: Distance polynomial and characterization of a graph, Natural Science Report, Ochanomizu University 24 (1973) 27-34.
- [b] D. Cvetkovič, M. Doob and H. Sachs: Spectra of graphs, Academic Press, Berlin 1983 (printed in GDR).

Souhrn

O DISTANČNÍM POLYNOMU GRAFU

PAVEL KŘIVKA, NENAD TRINAJSTIĆ

Článek se zabývá některými vlastnostmi distančního polynomu některých typů grafů, speciálně cest, bipartitních grafů, cyklů a hvězd.

Authors' addresses: RNDr. Pavel Křivka, CSc., Vysoká škola chemickotechnologická, Leninovo nám. 565, 532 10 Pardubice; Prof. Nenad Trinajstić, Rugjer Bošković Institute, P.O.B. 1016, 41001 Zagreb, Croatia Yugoslavia.