SOME GRAPH INVARIANTS RELATED TO THE DISTANCE MATRIX OF A DIGRAPH.

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Abstract: *It is the very usual case that the sbortest paths between all pairs of vertices in a given graph are required. Then the distance matrix D of such graph has to be arranged. In addition some quantities related to the distance matrix D can be useful. The program in the system Mathematica was created to calculate specific quantities for a given directed graph. Further the determinant of the distance matrix and the distance polynomial for a cycle with n vertices were found.*

Keywords: *Digraph, Distance Matrix, Distance Polynomial.*

1. Introduction

The graphs considered here are finite, directed and without loops and parallel (multiple) arcs (edges). A weighted digraph (directed graph) G is a digraph along with a mapping $c: A(G) \to R$, where $A(G)$ is the set of arcs of the digraph G. An unweighted digraph can be viewed as a weighted digraph with $c(a) = 1$ for any arc a of G. The other notations and terminology are as in the books [1] and [2].

Definition 1. *Let G be a weighted digraph with n vertices. Then the distance matrix of G is defined as n × n matrix D(G) = D = (d_{ij}), where*

$$d_{ij} = \begin{cases} \text{the distance from i to j,} \\ 0, \text{ if } i = j, \\ \text{if no path from i to j exists.} \end{cases}$$

The distance from i to j is the weight of the shortest path from i to j.

Definition 2. *Let D be the distance matrix of a digraph G. The distance polynomial of G is defined as* $P(G; x) = \det(xI - D)$ *, where I is the unit matrix of the size n × n.*

The distance matrix and the distance polynomial can be defined for undirected graphs in the same way.

The problem of finding of the distance matrix in a graph has a surprising variety of applications. An obvious example is the preparation of tables indicating distances between all pairs of major cities and towns in road maps of the state or region, which often accompany such maps. This type of computation is also virtually invariably required in all urban service system problems related to the location of urban facilities of the distribution on delivery of goods. It is therefore important to have available a highly efficient method for obtaining these shortest paths.

Křivka and Trinajstić dealt in [4] with the distance matrix and polynomial for simple undirected graphs. They obtained some interesting results.

Theorem 1 (**[4], Proposition 6**). *If there are two vertices with the same neighbourhood in a graph G, then one root of the distance polynomial* $P(G; x)$ *is either* -1 *(if the vertices are adjacent) or* -2 *(if the two vertices are not adjacent).*

Theorem 2 (**[4], Proposition 7**). *If G is a path on* $n+1$ *vertices* ($n \geq 3$)*, then* $a_0 = (-1)^n\, 2^{n-1}$*, where* a_0 *is a constant coefficient of* $P(G; x)$*, i. e.* $a_0 = det(-D)$.

Theorem 3 (**[4], Proposition 9**). *If G is a star with n vertices, then*

$$P(G; x) = (x + 2)^{n-2}\,(x^2 - 1 - (n-2)(2x + 1)) .$$

Theorem 4 ([4], Proposition 10). *If G is an circuit on n vertices, then at least one root of the distance polynomial* $P(G; x)$ *is zero.*

2. Program for calculation of the distance matrix and related quantities

First, we mention the most known algorithms. Almost all algorithms are for finding the distances from a fixed vertex of a digraph to the rest of the vertices. If the given digraph is unweighted then one can use the simple and fast breadth - first search algorithm. When G is an arbitrary digraph, but its weights are nonnegative, Dijkstra's algorithm solves the problem. When the weights may be negative, but no negative cycle is allowed, the Bellman-Ford-Moore algorithm can be applied. This algorithm has also the following additional useful property: it can be used to detect a negative cycle (if it exists). If we are interested in finding the distances between all pairs of vertices of a weighted digraph *G*, we can apply the previous algorithm from every vertex of *G*. Hovever, there is a much faster algorithm, due to Floyd and Warshall (more details in [6], pp. 45-58).

We used Floyd's algorithm to create a program for the calculation of the distance matrix of a weighted digraph. This is based on the system Mathematica for its good manipulation of ∞ and therefore the algorithm could be used simply enough. The language Pascal has been used with respect to need an interactive drawing of a given digraph. The program proceeds as follows.

```
MatrixAdjacencyToMatrixWeights::usage :=
"MatrixAdjacencyToMatrixWeights[m] computes the matrix D0 of weights
of arcs of the adjacency matrix for the related unweighted digraph."
```

FloydAM::usage := "FloydAM[mat] computes the distance matrix D of an arbitrary unweighted digraph given by its adjacency matrix."

FloydMW::usage := "FloydW[mat] computes the distance matrix D of an arbitrary weighted digraph given by its matrix D0."

```
MatrixAdjacencyToMatrixWeights[mat_]:=
Module[{m = mat,  n=Length[mat]}, Print[n];
     Do[
        If[i=!=j, If[ m[[i,j]] == 0, m[[i,j]] = Infinity ] ]
        ,{i,1,n},{j,1,n}
      ]; m
     ]

FloydAM[mat_]:=
 Module[ {m = MatrixAdjacencyToMatrixWeights[mat], n=Length[mat]},
       Do[
         Do[
           m[[i,j]] = Min[ m[[i,j]], m[[i,k]] + m[[k,j]]]
          ,{i,1,n},{j,1,n}
           ]
          , {k,1,n}
         ]; m
      ]

FloydMW[mat_]:=
 Module[ {m = mat, n=Length[mat]},
       Do[
         Do[
           m[[i,j]] = Min[ m[[i,j]], m[[i,k]] + m[[k,j]]]
          ,{i,1,n},{j,1,n}
           ]
          , {k,1,n}
         ]; m
      ]
```

For an illustration, the distance matrix and related invariants were calculated for the digraph in Figure 1.

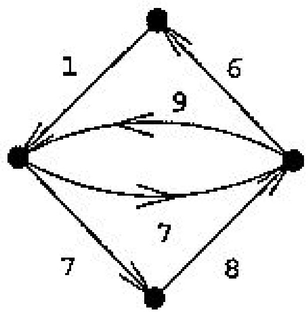

Fig. 1

$$D_0 = \begin{vmatrix} 0 & 1 & \infty & \infty \\ \infty & 0 & 7 & 7 \\ 6 & 9 & 0 & \infty \\ \infty & \infty & 8 & 0 \end{vmatrix}, \qquad D_3 = \begin{vmatrix} 0 & 1 & 8 & 8 \\ 13 & 0 & 7 & 7 \\ 6 & 7 & 0 & 14 \\ 14 & 15 & 8 & 0 \end{vmatrix}$$

det D = –27916,

eigenvalues {–8.558 – 6.007i, –8.558 + 6.007i, –9.569, 26.685},

$P(G;x) = x^4 - 439x^2 - 6242x - 27916$.

3. The case of a cycle

Gradshteyn and Ryzhik defined and expanded circulant matrices and their determinants.

Theorem 5 ([3], pp. 1111 - 1112). *Let* x_j, $j = 1, \ldots, n$, *be complex numbers. Then*

$$\begin{vmatrix} x_1 & x_2 & \ldots & x_n \\ x_n & x_1 & \ldots & x_{n-1} \\ & & \ldots & \\ x_2 & x_3 & \ldots & x_1 \end{vmatrix} = \prod_{j=1}^{n} (x_1 + x_2 e_j + x_3 e_j^2 + \mathbf{L} + x_n e_j^{n-1}),$$

where ε_j, $j = 1, \ldots, n$, *are the n-th roots of unity. The eigenvalues* λ_j *of the corresponding n × n circulant matrix are*

$$\lambda_j = x_1 + x_2\varepsilon_j + x_3\varepsilon_j^2 + \ldots + x_n\varepsilon_j^{n-1}.$$

Lemma. *Let* $\varepsilon \neq 1$ *be any complex number. Then*

$$\varepsilon + 2\varepsilon^2 + \ldots + n\varepsilon^n = \sum_{k=1}^{n} k\varepsilon^k = \frac{\varepsilon}{(1-\varepsilon)^2}\left(1-(n+1)\varepsilon^n + n\varepsilon^{n+1}\right).$$

Proof. The statement can be easy proved by induction on *n*.

It is more complicated to find the determinant of the distance matrix, the eigenvalues of this matrix or the distance polynomial for an arbitrary digraph. Therefore we will consider only a cycle C_n with *n* vertices as the case of the simplest strong connected digraph.

Theorem 6. *For a cycle* C_n *with* $n \geq 2$ *vertices the following statements hold.*

1.

$$\det D(C_n) = (-1)^{n-1}\binom{n}{2} n^{n-2},$$

2.

$$P(C_n; x) = \left(x - \binom{n}{2}\right)\prod_{j=2}^{n}\left(x - \frac{\varepsilon_j}{(1-\varepsilon_j)^2}\left(1 - n\varepsilon_j^{\,n-1} + (n-1)\varepsilon_j^{\,n}\right)\right),$$

where ε_j, $j = 1, \ldots, n$, *are the n-th roots of unity,*

3. the matrix $D(C_n)$ *has the eigenvalues*

$$x_1 = \binom{n}{2},\; x_j = \frac{\varepsilon_j}{(1-\varepsilon_j)^2}\left(1 - n\varepsilon_j^{\,n-1} + (n-1)\varepsilon_j^{\,n}\right),$$

for $2 \leq j \leq n$.

Proof. It is easy to see that the distance matrix for a cycle C_n has the form

$$D(C_n) = \begin{pmatrix} 0 & 1 & 2 & \ldots & n-1 \\ n-1 & 0 & 1 & \ldots & n-2 \\ & & \ldots\ldots & & \\ 1 & 2 & 3 & \ldots & 0 \end{pmatrix}.$$

1. $$det\ D(C_n) = \begin{vmatrix} 0 & 1 & 2 & 3 & \dots & n-1 \\ n-1 & 0 & 1 & 2 & \dots & n-2 \\ n-2 & n-1 & 0 & 1 & \dots & n-3 \\ & & & & \dots & \\ 1 & 2 & 3 & 4 & \dots & 0 \end{vmatrix}$$

First, we subtract the (k+1)-st row from the k-th, for k = 2, ..., n – 1, and the first row from the n-th. We get

$$\begin{vmatrix} 0 & 1 & 2 & 3 & \dots & n-1 \\ 1 & -(n-1) & 1 & 1 & \dots & 1 \\ 1 & 1 & -(n-1) & 1 & \dots & 1 \\ & & & & \dots\dots & \\ 1 & 1 & 1 & 1 & \dots & -(n-1) \end{vmatrix}$$

Afterwards we subtract the first column from all the following ones

$$\begin{vmatrix} 0 & 1 & 2 & 3 & \dots & n-1 \\ 1 & -n & 0 & 0 & \dots & 0 \\ 1 & 0 & -n & 0 & \dots & 0 \\ & & & & \dots & \\ 1 & 0 & 0 & 0 & \dots & -n \end{vmatrix}$$

and finally expand with respect to the first row. Then

$$\det D(C_n) = -1(-n)^{n-2} - 2(-n)^{n-2} - \mathbf{L} - (n-1)(-1)^{n-2} = (-1)^{n-1}\binom{n}{2}n^{n-2}.$$

2. By Definition 2 and using Theorem 5 we get

$$P(C_n;x) = \begin{vmatrix} x & -1 & -2 & \dots & -(n-1) \\ -(n-1) & x & -1 & \dots & -(n-2) \\ & & \dots\dots & & \\ -1 & -2 & -3 & \dots & x \end{vmatrix} =$$

$$= \prod_{j=1}^{n}.(x - e_j - 2e_j^{\,2} - \mathbf{L} - (n-1)e_j^{\,n-1}) = \prod_{j=1}^{n}(x - \sum_{k=1}^{n-1} ke_j^{\,k}).$$

As one of the root of unit equals 1 for any positive integer n (e.g. $e_1 = 1$) we can write

$$P(C_n; x) = \left(x - \sum_{k=1}^{n-1} k \right) \prod_{j=2}^{n-1} \left(x - \prod_{k=1}^{n-1} k e_j^{\,k} \right).$$

Using Lemma we have

$$P(C_n; x) = \left(x - \binom{n}{2} \right) \prod_{j=2}^{n} \left(x - \frac{e_j}{(1-e_j)^2} (1 - n e_j^{\,n-1} + (n-1) e_j^{\,n} \right).$$

3. We obtain eigenvalues immediately as the roots of the distance polynomial from its expression in the previous factorization.

Table 1: The distance polynomial $P(C_n; x)$ of a cycle C_n and the determinant of the distance matrix $D(C_n)$ for small values n

n	$P(C_n; x)$	$\det D(C_n)$
2	$(x - 1)(x + 1)$	–1
3	$(x - 3)(x^2 + 3x + 3)$	6
4	$(x - 6)(x + 2)(x^2 + 4x + 8)$	–96
6	$(x - 15)(x + 9)(x^2 + 6x + 36)(x^2 + 6x + 12)$	–19 440

It is obvious from Theorem 6 that only one eigenvalues is real for odd *n* and just two eigenvalues are real for even *n*.

4. Concluding remarks

After small arrangement the created program works for undirected graphs, too. Then the distance matrix can be used to compute another useful invariants of a graph *G*, that are related to the center of *G*. These invariants are for example the eccentricity of a vertex in *G*, the radius and the diameter of a graph *G* or Wiener's index which is defined as the sum of all nondiagonal entries of the distance matrix. This index is often used in chemistry.

From the mathematical point of view the main result of this contribution is the calculation of invariants related to the distance matrix for a directed cycle with n vertices. An interesting problem is also to investigate properties of these invariants for other classes of strong connected digraphs, such as distance--regular graphs, strong tournaments and so on. We found in [5] some invariants for digraphs with the companion matrix as their adjacency matrix.

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