

Bogusław Gąsiorowski, Michał Rozmus

APPLICATION OF THE CHARACTERISTIC POLYNOMIAL OF THE TRANSITION MATRIX TO THE INVESTIGATION OF THE PROPERTIES OF A FINITE GRAPH

D e f i n i t i o n 1. We call a finite multigraph the triplet $G = (X, U, R)$, where:
 $|X| < +\infty$; X is the set of vertices of the multigraph,
 $|U| < +\infty$; U is the set of branches of the multigraph,
 $R \subset (X, U, X)$,

the following conditions being satisfied:

- 1) to any $u \in U$ there exist $x, y \in X$ such that $(x, u, y) \in R$,
- 2) to any $u \in U$ if there exist $x, y, z, k \in X$, such that $(x, u, z) \in R$ and $(y, u, k) \in R$, then $x = y$ and $z = k$ or $x = k$ and $y = z$.

D e f i n i t i o n 2. In the finite multigraph $G = (X, U, R)$ the branch $u \in U$ is said to be
a) a loop, if there exists an $x \in X$ such that $(x, u, x) \in R$,
b) an arc, if there exist $x, y \in X$ such that $(x, u, y) \in R$, $(y, u, x) \notin R$,
c) an edge, if there exist $x, y \in X$ such that $(x, u, y) \in R$ and $(y, u, x) \in R$.

In what follows we shall consider finite multigraphs without loops.

To any finite multigraph we can give a geometrical interpretation in the following way:

- 1) to each vertex $x \in X$ we assign a point x of the plane, so that to distinct vertices are assigned distinct points,

- 2) to each arc $u \in U$ such that $(x, u, y) \in R$ we assign in the plane a segment directed from the point x to the point y .
- 3) to each edge $u \in U$ such that $(x, u, y) \in R$ we assign in the plane an undirected segment joining the points x and y .

A multigraph containing no edges (arcs) is said to be directed (undirected).

If in a multigraph any pair of vertices are joined by no more than one branch, the multigraph is called a graph. In particular, a graph cannot contain arcs joining the same vertices and reversely directed.

We call route of length l with origin x_{i_0} and end x_{i_l} an alternate sequence of vertices and branches of the multigraph of the form $\{x_{i_0}, u_{i_1}, x_{i_1}, u_{i_2}, \dots, u_{i_l}, x_{i_l}\}$, such that for any $k = 1, \dots, l$ the branch u_{i_k} joins the vertices $x_{i_{k-1}}$ and x_{i_k} (if u_{i_k} is an arc, then it may be directed from $x_{i_{k-1}}$ to x_{i_k} or reversely). A route of length l such that all the branches are distinct is said to be a chain of length l .

A chain whose each arc u_{i_k} is directed from $x_{i_{k-1}}$ to x_{i_k} is said to be a path. A chain (route, path) whose all vertices are distinct is said to be simple. A chain (route, path) which begins and ends at the same vertex is called a cycle (cyclic route, cyclic path). A cycle (cyclic path) of length l , having l distinct vertices is called a simple cycle (simple cyclic path) of length l . A multigraph is said to be connected if to any pair of its vertices $x, y \in X$ there exists a chain with origin x and end y .

Definition 3. Let $X = \{x_1, x_2, \dots, x_n\}$ be the set of vertices of a finite multigraph $G = (X, U, R)$. We call a transition matrix $P = [p_{i,j}]$ the matrix such that

$$p_{i,j} = \left| \left\{ u \in U / (x_i, u, x_j) \in R \right\} \right| \quad \text{for } i, j = 1, \dots, n.$$

Definition 4. a) The metric of the multigraph $G = (X, U, R)$ is defined as the function

$$\rho(x, y) = \begin{cases} 0, & \text{if } x = y, \\ +\infty, & \text{if } x \neq y \text{ and if there exists no chain with} \\ & \text{origin } x \text{ and end } y, \\ 1, & \text{otherwise,} \end{cases}$$

where 1 denotes the length of the shortest chain with origin x and end y .

b) The vertex $x_0 \in X$ is said to be: central, if for any $x \in X$ $\max_{y \in X} \rho(x_0, y) \leq \max_{y \in X} \rho(x, y)$ or peripheral, if for any $x \in X$ $\max_{y \in X} \rho(x_0, y) \geq \max_{y \in X} \rho(x, y)$.

c) The radius of the multigraph is defined as the number

$$r(G) = \min_{x \in X} \max_{y \in X} \rho(x, y).$$

The diameter of the multigraph is defined as the number

$$d(G) = \max_{x, y \in X} \rho(x, y).$$

d) Let $A, B \subset X$, $A \neq \emptyset$, $B \neq \emptyset$. The distance between the sets A, B is defined as the number

$$\rho(A, B) = \min_{\substack{x \in A \\ y \in B}} \rho(x, y).$$

The distance of the vertex x_0 to the set A is defined as the number

$$\rho(x_0, A) = \min_{y \in A} \rho(x_0, y).$$

In what follows we shall assume that

$G = (X, U, R)$ is a finite multigraph without loops,

$X = \{x_1, x_2, \dots, x_n\}$;

Let us now denote by:

a) $D_{i,k}^*$: $k = 2, \dots, n$; $i = 1, \dots, \left\lfloor \frac{k}{2} \right\rfloor$, the set whose elements are i sets of cyclic simple paths without common vertices, such that the sum of their lengths equals k . In special cases, for some i, k the set $D_{i,k}^*$ may be empty.

b) $P = P(G)$ the transition matrix for G , with the assumed numbering of vertices.

c) $D_{i,j}(\lambda)$ the co-factor of the element in the i -th row and j -th column of the matrix $P - \lambda E$; $D_{i,j}(\lambda)$ is a polynomial of degree $k_{i,j}$ in the variable λ , such that the highest power of λ has the coefficient $H_{i,j}$.

R e m a r k 1. Given a multigraph G it is possible to build:

a) a directed multigraph $G_1 = (X, U_1, R_1)$ in such a way that each edge of G joining the vertices x and y is replaced by the pair of reversely directed arcs in G_1 which join the same vertices,

b) a directed multigraph $G_2 = (X, U_2, R_2)$ with a symmetrical transition matrix, in such a way that to each branch of G joining the vertices x, y there corresponds in G_2 exactly one pair of reversely directed arcs joining these vertices. It is easy to see that to each path in G there corresponds in G_1 exactly one path passing through the same vertices. The transition matrices for G and G_1 are identical and the transition matrix of G_2 is symmetrical.

Let us now recall the following theorem (see [1]):

T h e o r e m 1. The characteristic polynomial of the matrix P is

$$\det(P - \lambda E) = (-1)^n (\lambda^n + a_2 \lambda^{n-2} + a_3 \lambda^{n-3} + \dots + a_n),$$

where, for any $k = 2, \dots, n$:

$$a_k = -|D_{1,k}^*| + |D_{2,k}^*| - |D_{3,k}^*| + \dots + (-1)^{\left\lfloor \frac{k}{2} \right\rfloor} |D_{\left\lfloor \frac{k}{2} \right\rfloor, k}^*|.$$

Theorem 2. Let G_1 be a directed multigraph corresponding to G in accordance with Remark 1.

Let be given the sets of vertices:

$$X_1 = \{x_{j_1}, x_{j_2}, \dots, x_{j_r}\} \subset X; \quad r \geq 1,$$

$$X_2 = \{x_{i_1}, x_{i_2}, \dots, x_{i_s}\} \subset X; \quad s \geq 1,$$

$$X_1 \cap X_2 = \emptyset.$$

Denote:

a) by $G_3 = (X, U_3, R_3)$ the multigraph obtained from G_1 in the following way: for each pair of vertices $(x_{i_k}, x_{j_w}) \in X_2 \times X_1$ we remove in G_1 all the arcs joining x_{i_k} with x_{j_w} , then we join them by exactly one arc,

b) by $G_4 = (X, U_4, R_4)$ the directed multigraph obtained from G_1 by removing from U_1 the arcs joining vertices which belong to the set X_2 with the vertices of set X_1 ,

c) by P_3, P_4 the transition matrices for G_3 and G_4 respectively,

d) by $W(\lambda) = \det(P_3 - \lambda E) - \det(P_4 - \lambda E)$ a polynomial in the variable λ of degree $k_1(X_1, X_2)$ such that the coefficient of the highest power of λ equals $H(X_1, X_2)$.

A s s e r t i o n . 1) A necessary and sufficient condition in order that there exist in G a path whose origin belongs to X_1 and end belongs to X_2 is that $W(\lambda) \neq 0$.

2) If $W(\lambda) \neq 0$, then the shortest of these paths has the length $n-1-k(X_1, X_2)$. The number of these shortest paths is $|H(X_1, X_2)|$.

P r o o f . By Theorem 1 we have

$$(A) \begin{cases} \det(P_3 - \lambda E) = (-1)^n (\lambda^n + (a_2)_3 \lambda^{n-2} + (a_3)_3 \lambda^{n-3} + \dots + (a_n)_3) \\ \det(P_4 - \lambda E) = (-1)^n (\lambda^n + (a_2)_4 \lambda^{n-2} + (a_3)_4 \lambda^{n-3} + \dots + (a_n)_4), \end{cases}$$

where for each $r = 2, \dots, n$

$$(B) \quad \begin{cases} (a_r)_3 = -|D_{1,r}^*|_3 + |D_{2,r}^*|_3 - |D_{3,r}^*|_3 + \dots + (-1)^{\left[\frac{r}{2}\right]} |D_{\left[\frac{r}{2}\right],r}^*|_3 \\ (a_r)_4 = -|D_{1,r}^*|_4 + |D_{2,r}^*|_4 - |D_{3,r}^*|_4 + \dots + (-1)^{\left[\frac{r}{2}\right]} |D_{\left[\frac{r}{2}\right],r}^*|_4. \end{cases}$$

We shall restrict ourselves to simple paths, since the shortest paths are always simple ones. G_4 is a partial multi-graph of G_3 , obtained by removing from the set U_3 the subset

$$U_{1,3} = \left\{ u \in U_3 / (x_{1_k}, u, x_{j_w}) \in R_3; \quad x_{1_k} \in X_2; \quad x_{j_w} \in X_1 \right\}.$$

All the simple cyclic paths belonging to G_3 and not belonging to G_4 are obtained by composing the simple paths joining the vertices of X_1 with the vertices of X_2 with the corresponding arcs of the set $U_{1,3}$. The multigraph G does not contain paths joining the vertices of X_1 and X_2 if and only if all the sets of simple cyclic paths in G_3 and G_4 are identical. Hence

$$|D_{i,r}^*|_3 = |D_{i,r}^*|_4 \quad \text{for } r = 2, \dots, n; \quad i = 1, \dots, \left[\frac{r}{2}\right].$$

By (A) and (B) this is equivalent to the equality $W(\lambda) = 0$.

Suppose that $W(\lambda) \neq 0$ and that k denotes the least length of a cyclic path belonging to G_3 and not belonging to G_4 we have

$$|D_{i,r}^*|_3 = |D_{i,r}^*|_4 \quad \text{for } 2 \leq r < k,$$

$$(a_r)_3 = (a_r)_4 \quad \text{for } 2 \leq r < k.$$

Moreover,

$$\left| (a_k)_4 - (a_k)_3 \right| = \left| \left| D_{1,k}^* \right|_4 - \left| D_{1,k}^* \right|_3 \right|,$$

since

$$\left| D_{i,k}^* \right|_3 = \left| D_{i,k}^* \right|_4 \quad \text{for } i \geq 2.$$

The length of the shortest path whose origin belongs to X_1 and end belongs to X_2 is $k-1$ and the number of such paths equals

$$\left| \left| D_{1,k}^* \right|_4 - \left| D_{1,k}^* \right|_3 \right| = \left| (a_k)_4 - (a_k)_3 \right| = \left| H(X_1, X_2) \right|$$

$$k-1 = n-1 - k(X_1, X_2).$$

T h e o r e m . If G is an undirected graph, then for all $x, y \in X$ there exists in G exactly one shortest path joining these vertices if and only if

$$D_{i,j}(\lambda) \neq 0, \quad |H_{i,j}| = 1 \quad \text{for } i, j=1, \dots, n; \quad i > j.$$

P r o o f . When building the directed multigraph G_1 corresponding to G by Remark 1, it should be noted that the matrix P_1 for G_1 is identical with the matrix P for G . Since the matrix P is symmetrical, we have merely to consider the case $i > j$. The above theorem follows directly from Theorem 2 for $r = 1$ and $s = 1$, if we make use of the true equality

$$W(\lambda) = D_{i_1, j_1}(\lambda) = D_{j_1, i_1}(\lambda).$$

The theorem yields in algebraic form the solution of a problem stated by Ore (see [3], p.119): "Describe the class of undirected graphs such that for any pair of vertices x, y there

exists exactly one shortest path joining them". This problem has been till now solved only for planar graphs (see [2]).

In what follows we shall assume that:

- a) $G_2 = (X, U_2, R_2)$ is a directed multigraph constructed for G in accordance with Remark 1.
- b) P_2 is the transition matrix for G_2 ,
- c) for any $i, j = 1, \dots, n$: $D_{i,j}^2(\lambda)$ denotes the co-factor of the element in the i -th row and j -th column of the matrix $P_2 - \lambda E$,
- d) $k_{i,j}^2$ denotes the degree of the polynomial $D_{i,j}^2(\lambda)$ in the variable λ .

Theorem. If G is a connected multigraph, $|X| \geq 2$, then:

- 1) The radius of the multigraph is

$$r(G) = n - 1 - \max_{i \neq j} \min_{n \geq i \geq 1} k_{i,j}^2.$$

- 2) The diameter of the multigraph is

$$d(G) = n - 1 - \min_{n \geq i > j \geq 1} k_{i,j}^2.$$

- 3) If $x_i \in X$, then

- 3a) x_i is a central vertex if and only if for any $r = 1, \dots, n$

$$\min_{\substack{r \neq j \\ j=1, \dots, n}} k_{r,j}^2 \leq \min_{\substack{i \neq j \\ j=1, \dots, n}} k_{i,j}^2$$

- 3b) x_i is a peripheral vertex if and only if the inequality under 3a) is replaced either by the reverse inequality or by the equality.

Proof. 1) Since $|X| \geq 2$, there exists for each i ; $j \neq i$ such that $\rho(x_i, x_j) > 0$. We have merely to consider the case $i \neq j$.

Since G is connected, so is G_2 and

$$D_{i,j}^2(\lambda) \neq 0 \quad \text{for } i, j = 1, \dots, n, \quad i \neq j.$$

$$r(G) = \min_{i \neq j} \max_{i=1, \dots, n} \rho(x_i, x_j) = n - 1 - \max_{n \geq i \neq j} \min_{n \geq j \geq 1} k_{i,j}^2.$$

2) The proof is similar to that of case 1).

3) x_i is a central vertex if and only if for each $x_r \in X$ the following inequality holds

$$(A) \quad \max_{j=1, \dots, n} \rho(x_i, x_j) \leq \max_{h=1, \dots, n} \rho(x_r, x_h).$$

Similarly to case 1) we can restrict ourselves to the case $i \neq j, h \neq r$ we have

$$\rho(x_i, x_j) = n - 1 - k_{i,j}^2$$

$$\rho(x_r, x_h) = n - 1 - k_{r,h}^2.$$

Hence the inequality (A) is equivalent to the inequality

$$\left\{ \min_{\substack{i \neq j \\ j=1, \dots, n}} k_{i,j}^2 \right\} \geq \left\{ \min_{\substack{r \neq j \\ j=1, \dots, n}} k_{r,j}^2 \right\}.$$

3b) The proof is analogous to that of case 3a).

Theorem. Let $r \geq 2$ and $x_{i_1}, x_{i_2}, \dots, x_{i_r}$ be a sequence of vertices of the multigraph G such that $x_{i_{l+1}} \neq x_{i_l}$ for $l = 1, \dots, r-1$.

Assertion. 1) A directed route from x_{i_1} to x_{i_r} passing in turn through the vertices $x_{i_2}, x_{i_3}, \dots, x_{i_{r-1}}$ exists if and only if

$$\left| \prod_{l=2}^r D_{i_l, i_{l-1}}(\lambda) \right| \neq 0.$$

2) If condition 1) is satisfied, then there exist in G exactly $\prod_{l=2}^r |H_{i_l, i_{l-1}}|$ directed routes with origin x_{i_1} and end x_{i_r} passing through the vertices $x_{i_2}, x_{i_3}, \dots, x_{i_{r-1}}$ and having the least length; the length of each of them is

$$(r-1)(n-1) - \sum_{l=2}^r k_{i_l, i_{l-1}}.$$

P r o o f . To obtain the shortest route wanted in the theorem we compose the shortest paths joining the vertices x_{i_1} with x_{i_2} , x_{i_2} with $x_{i_3}, \dots, x_{i_{r-1}}$ with x_{i_r} . Applying Theorem 2 to the paths that form this route and making use of the equality

$$W_l(\lambda) = D_{i_l, i_{l-1}}(\lambda) \quad \text{for } l=1, \dots, r-1$$

we get the assertion.

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INSTITUTE OF MATHEMATICS, SILESIAN TECHNICAL UNIVERSITY, GLIWICE
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