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On Path Eigenvalues and Path Energy of Graphs

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Abstract

Given a graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, we associate to G a path matrix $\mathbf{P}$ whose (i, j)-entry is the maximum number of vertex disjoint paths between the vertices v_i and v_j when $i \neq j$ and is zero when $i = j$. We explore some properties of the eigenvalues and energy of $\mathbf{P}$.

1 Introduction

For a graph G, the eigenvalues of G are the eigenvalues of its adjacency matrix, forming the spectrum of G. For details of the spectral theory we refer to the seminal monograph by Cvetković et al. [7], as well as to [2,6,8,19]. For undefined terminology and notations, see [4,20].

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Define the matrix $\mathbf{P} = (p_{ij})$ of size $n \times n$ such that p_{ij} is equal to the maximum number of vertex disjoint paths from v_i to v_j if $i \neq j$, and $p_{ij} = 0$ if $i = j$.

We say that $\mathbf{P} = \mathbf{P}(G)$ is the *path matrix* of the graph G [16]. By definition, $\mathbf{P}$ is a real and symmetric matrix. Therefore, its eigenvalues are real. We call the eigenvalues of $\mathbf{P}$ the *path eigenvalues* of G, forming its *path spectrum* $\mathrm{Spec}_{\mathbf{P}}(G)$.

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For convenience, the eigenvalues of the adjacency matrix of G will be referred to as the ordinary eigenvalues of G, forming its ordinary spectrum Spec(G) [7,8].

Consider the graph G shown in Fig. 1. Its path matrix is:

$$\mathbf{P}(G) = \begin{bmatrix} 0 & 2 & 2 & 1 & 1 & 1 & 1 \\ 2 & 0 & 2 & 1 & 1 & 1 & 1 \\ 2 & 2 & 0 & 2 & 2 & 2 & 1 \\ 1 & 1 & 2 & 0 & 3 & 2 & 1 \\ 1 & 1 & 2 & 3 & 0 & 2 & 1 \\ 1 & 1 & 2 & 2 & 2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}.$$

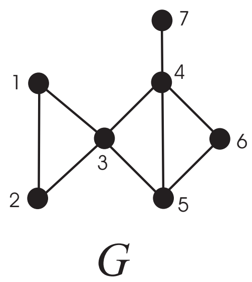

Fig. 1. A graph whose vertices 1 and 6 are connected by eight paths (1346, 13456, 1356, 13546, 12346, 123456, 12356, 123546) of which no two are vertex disjoint; therefore $p_{16}(G) = 1$.

The path spectrum of the graph G from Fig. 1 is

$$\mathrm{Spec}_{\mathbf{P}}(G) = \{9.1136, 0.7143, -0.6604, -2.4781, -2.0000, -1.6894, -3.0000\}$$

whereas its ordinary spectrum is

$$\mathrm{Spec}(G) = \{2.9240, 1.5760, 0.3149, -0.5289, -1.0000, -1.3363, -1.9497\}\,.$$

2 Properties of path eigenvalues of graphs

Denote by $\mathbf{J}_n$ the square matrix of order n, whose all non-diagonal elements are equal to one, and all diagonal elements are zero. Note that this is just the adjacency matrix of the complete graph K_n. Its spectrum is known to be [7,8]

$$\mathrm{Spec}(K_n) = \{n-1, -1, -1, \ldots, -1\}\,.$$

Example 1. *Let T be a tree of order n. Then for any $v_i, v_j \in V(T)$, $i \neq j$, there is a single path connecting v_i and v_j. Therefore, $\mathbf{P}(T) = \mathbf{J}_n$ and*

$$Spec_{\mathbf{P}}(T) = \{n-1, -1, -1, \ldots, -1\}\,.$$

Example 2. *Let C_n be the cycle of order n. Then for any $v_i, v_j \in V(T)$, $i \neq j$, there are two vertex disjoint paths connecting v_i and v_j. Therefore, $\mathbf{P}(C_n) = 2\,\mathbf{J}_n$ and*

$$Spec_{\mathbf{P}}(C_n) = \{2(n-1), -2, -2, \ldots, -2\}\,.$$

Denote by $\mathbf{1}$ a matrix of appropriate dimensions, whose all elements are equal to 1.

Example 3. *Let $U_{n,k}$ be a unicyclic graph of order n whose cycle is of size k. Then the vertices of $U_{n,k}$ can be labeled so that*

$$\mathbf{P}(U_{n,k}) = \begin{bmatrix} \mathbf{P}(C_k) & \mathbf{1} \\ \mathbf{1} & \mathbf{J}_{n-k} \end{bmatrix} = \begin{bmatrix} 2\,\mathbf{J}_k & \mathbf{1} \\ \mathbf{1} & \mathbf{J}_{n-k} \end{bmatrix}.$$

Example 4. *Let K_n be the complete graph of order n. Then for any $v_i, v_j \in V(K_n)$, $i \neq j$, there are $n-1$ vertex disjoint paths connecting v_i and v_j. For instance, if $i = 1$ and $j = 2$, these paths are: 12, 132, 142, 152, $\ldots, 1n2$. Therefore, $\mathbf{P}(K_n) = (n-1)\mathbf{J}_n$ and*

$$Spec_{\mathbf{P}}(K_n) = \{(n-1)^2, -(n-1), -(n-1), \ldots, -(n-1)\}\,.$$

Example 5. *Let $K_{h,\ell}$, $h \leq \ell$ be the complete bipartite graph on $h + \ell$ vertices, and let $x_1, x_2, \ldots, x_h$ be the vertices of its one part and $y_1, y_2, \ldots, y_\ell$ of the other part. Then there are ℓ vertex disjoint paths connecting the vertices x_i and x_j:*

$$x_i y_1 x_j \ , \ x_i y_2, x_j \ , \ x_i y_3 x_j \ , \ldots , \ x_i y_\ell x_j$$

and, analogously, h vertex disjoint paths connecting the vertices y_i and y_j. On the other hand, there are h vertex disjoint paths connecting x_i and y_j. For instance, if $i = j = 1$, then these are

$$x_1 y_1 \ , \ x_1 y_2 x_2 y_1 \ , \ x_1 y_3 x_3 y_1 \ , \ldots , \ x_1 y_h x_h y_1\,.$$

Therefore,

$$\mathbf{P}(K_{h,\ell}) = \begin{bmatrix} \ell\,\mathbf{J}_h & h\,\mathbf{1} \\ h\,\mathbf{1} & h\,\mathbf{J}_\ell \end{bmatrix}.$$

If $h = \ell$, then $\mathbf{P}(K_{h,h}) = h\,\mathbf{J}_{2h}$ and

$$Spec_{\mathbf{P}}(K_{h,h}) = \{h(2h-1), -h, -h, \ldots, -h\}\,.$$

The above examples show that the path spectrum may possess just a single positive eigenvalue. In the general case, however, the number of positive path eigenvalues may be greater than unity, even in the case of connected graphs. One such example is the graph G depicted in Fig. 1.

Proposition 1. *If the vertices v_i and v_j belong to two disconnected components of the graph G, then, evidently, $p_{ij} = 0$. Therefore, if G consists of components G_1 and G_2, then*

$$\mathbf{P}(G) = \begin{bmatrix} \mathbf{P}(G_1) & \mathbf{0} \\ \mathbf{0} & \mathbf{P}(G_2) \end{bmatrix}$$

and, consequently,

$$Spec_{\mathbf{P}}(G) = Spec_{\mathbf{P}}(G_1) \cup Spec_{\mathbf{P}}(G_2) \,.$$

Analogously, if G consists of $p \geq 2$ components $G_1, G_2, \ldots, G_p$, then

$$\mathbf{P}(G) = \begin{bmatrix} \mathbf{P}(G_1) & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{P}(G_2) & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{P}(G_p) \end{bmatrix}$$

and

$$Spec_{\mathbf{P}}(G) = \bigcup_{i=1}^{p} Spec_{\mathbf{P}}(G_i) \,.$$

Proposition 2. *Every integer is a path eigenvalue of some graph.*

Proof. Let k be an integer. If $k = 0$, then consider the null graph (the graph without edges). The path eigenvalues of the null graph are all zero.

Suppose that $k > 0$. Let T be a tree with $k+1$ vertices. Then k is a path eigenvalue of T.

Suppose that $k < 0$ and $k = -h$ where $h > 0$. Consider the complete bipartite graph $K_{h,h}$. Then $k = -h$ is a path eigenvalue of $K_{h,h}$. ■

For matrices $\mathbf{A} = (a_{ij})$ and $\mathbf{B} = (b_{ij})$, $\mathbf{A} \geq \mathbf{B}$ denotes $a_{ij} \geq b_{ij}$ for all i, j. If $\mathbf{A} \geq \mathbf{B}$ and $a_{ij} > b_{ij}$ for at least one i, j, then we write $\mathbf{A} > \mathbf{B}$.

Proposition 3. *Let G be a graph in which the vertices v_i and v_j are not adjacent. Let $G + e_{ij}$ be the graph obtained from G by connecting its vertices v_i and v_j. Then*

$$\mathbf{P}(G + e_{ij}) > \mathbf{P}(G) \,.$$

Proof. The transformation $G \to G+e_{ij}$ either increases or leaves unchanged the maximum number of vertex disjoint paths between any two vertices. In addition, $p_{ij}(G+e_{ij}) = p_{ij}(G)+1$. ■

Proposition 4. *Let G be a graph with vertex set $V(G)$. Denote by $d(v_i)$ the degree (number of first neighbors) of the vertex $v_i \in V(G)$. Then for all $v_i, v_j \in V(G)$,*

$$p_{ij}(G) \leq \min\left\{d(v_i), d(v_j)\right\}.$$

Proof. The number of vertex disjoint paths starting at a vertex v cannot be greater than $d(v)$. ■

Examples 2, 4, 5 show that there are graphs G for which the equality

$$p_{ij}(G) = \min\left\{d(v_i), d(v_j)\right\}$$

holds for all $v_i, v_j \in V(G)$. Using the notation defined below in Section 3, more such graphs are those of the form $pr^*(G)$ for $G \in \mathcal{B}^{(2)}$ and $G \in \mathcal{B}^{(3)}$, but not for $G \in \mathcal{B}^{(1)}$.

In what follows we state results for the path matrix that by the Perron–Frobenius theorem hold for any real square matrix with positive entries [10, 12, 15].

Theorem 1. *Let G be a connected graph with $n \geq 2$ vertices, and let $\mathbf{P}$ be the corresponding path matrix. Then the following statements hold:*
(i) $\mathbf{P}$ is irreducible.
(ii) $\mathbf{P}$ has a path eigenvalue $\rho = \rho(G) > 0$ and an associated eigenvector $\mathbf{x} > 0$. This eigenvalue will be referred to as the path spectral radius of the underlying graph G.
(iii) For any eigenvalue $\mu \neq \rho$ of $\mathbf{P}$, $-\rho \leq \mu \leq \rho$.
(iv) If $\mathbf{u}$ is an eigenvector of $\mathbf{P}$ for the path eigenvalue ρ, then $\mathbf{u} = \alpha\,\mathbf{x}$ for some α.

The next lemma is also a well known result of linear algebra.

Lemma 1. *If $\mathbf{A} \geq \mathbf{B}$ are non-negative matrices and $\mathbf{A}$ is irreducible, then $\rho(\mathbf{A}) > \rho(\mathbf{B})$.*

Combining Lemma 1 and Proposition 3 we directly arrive at:

Theorem 2. *Let G and $G+e_{ij}$ be the graphs specified in Proposition 3. If G is a connected graph, then $\rho(G+e_{ij}) > \rho(G)$.*

Corollary 1. *Let G be a connected graph of order n.*

(i) $\rho(G) \geq (n-1)$, with equality if and only if G is a tree of order n.

(ii) $\rho(G) \leq (n-1)^2$, with equality if and only if $G \cong K_n$.

Corollary 2. *Let G be a connected graph on n vertices, and let $H \neq G$ be a spanning, connected subgraph of G. Then $\rho(G) > \rho(H)$.*

Corollary 3. *Let G be a connected graph on n vertices and let H be an induced subgraph of G on n' vertices where $n' < n$. Then $\rho(G) > \rho(H)$.*

Corollary 4. *Let G be a connected graph on n vertices and let $H \neq G$ be a subgraph of G. Then $\rho(G) > \rho(H)$.*

Proposition 5. *Let G be a k-connected graph on $2k+1$ vertices. Then the path spectral radius of G lies in the interval $(4k, 4k^2)$.*

Proof. We know that a k-connected graph of order $2k+1$ contains a cycle of length $2k+1$. Thus G contains a cycle of order $2k+1$ and G is a subgraph of K_{2k+1}, the complete graph on $2k+1$ vertices. Therefore, $\mathbf{P}(C_{2k+1}) \leq \mathbf{P}(G)$ and $\mathbf{P}(G) \leq \mathbf{P}(K_{2k+1})$. This implies that $\mathbf{P}(C_{2k+1}) \leq \mathbf{P}(G) \leq \mathbf{P}(K_{2k+1})$. By Theorem 2 and its corollaries, $\rho(C_{2k+1}) < \rho(G) < \rho(K_{2k+1})$, that is $2(2k) < \rho(G) < (2k)^2$. Hence $\rho(G) \in (4k,\ 4k^2)$. ■

For $\mathbf{x} \in \mathbb{R}^n$, let $x_{[1]} \geq \cdots \geq x_{[n]}$ be a rearrangement of the coordinates of $\mathbf{x}$ in non-increasing order. If $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ then $\mathbf{x}$ is said to be *majorized* by $\mathbf{y}$, denoted $\mathbf{x} \prec \mathbf{y}$, if the following conditions hold:

$$\sum_{i=1}^{k} x_{[i]} \leq \sum_{i=1}^{k} y_{[i]} \quad \text{for} \;\; i = 1, \ldots, n-1$$

and

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \, .$$

An $n \times n$ matrix $\mathbf{A} = (a_{ij})$ is said to be doubly stochastic if $a_{ij} \geq 0$ for all i, j, and the row and the column sums of $\mathbf{A}$ are all equal to 1. The following result is proved in [2].

Lemma 2. *Let $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$. Then $\boldsymbol{x} \prec \boldsymbol{y}$ if and only if there exists an $n \times n$ doubly stochastic matrix $\mathbf{A}$ such that $\boldsymbol{x} = \mathbf{A}\boldsymbol{y}$.*

In the following Theorem 3, we prove that the vector of diagonal elements of $\mathbf{P}$ is majorized by the vector of path eigenvalues.

Theorem 3. *Let G be a graph on n vertices and let $\mathbf{P} = (p_{ij})$ be its path matrix. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the path eigenvalues of G. Then $(p_{11}, p_{22}, \ldots, p_{nn}) \prec (\lambda_1, \lambda_2, \ldots, \lambda_n)$.*

Proof. First recall that $(p_{11}, p_{22}, \ldots, p_{nn}) = (0, 0, \ldots, 0)$, that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and $\sum_{i=1}^{n} \lambda_i = 0$.

There exists an orthogonal matrix $\mathbf{A} = (a_{ij})$ such that

$$\mathbf{P} = \mathbf{A} \begin{bmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & \lambda_n \end{bmatrix} \mathbf{A}^t.$$

Hence,

$$p_{ii} = \sum_{j=1}^{n} a_{ij}^2 \, \lambda_j \quad \text{for} \quad i = 1, 2, \ldots, n. \tag{1}$$

Since $\mathbf{A}$ is orthogonal, the $n \times n$ matrix with (i, j)-element a_{ij}^2 is doubly stochastic. The result follows from Eq. (1) and Lemma 2. ■

3 Path spectral radius of unicyclic and bicyclic graphs

Let G be a graph. Assume that G is connected and that G is not a tree. Denote by $pr(G)$ the graph obtained by deleting from G all pendent vertices. Thus pr is a "pruning operation". If G has no pendent vertices, then $pr(G) \cong G$.

If $pr(G)$ still possesses pendent vertices, then repeat the pruning operation as many times as necessary until the resulting graph $pr^*(G)$ is free of pendent vertices. Assuming that $pr^*(G)$ has n^* vertices, the path matrix of G is then of the form:

$$\mathbf{P}(G) = \begin{bmatrix} \mathbf{P}(pr^*(G)) & \mathbf{1} \\ & \\ \mathbf{1} & \mathbf{J}_{n-n^*} \end{bmatrix}.$$

In what follows, we state a few results on the path spectral radius ρ of unicyclic and bicyclic graphs. These all are immediate special cases of Lemma 1, Theorem 2, and its corollaries.

3.1 Unicyclic graphs

Denote by C_p the cycle on p vertices. Denote by $\mathcal{U}_n$ the set of connected unicyclic graphs with n vertices. Let, in addition, $\mathcal{U}_{n,k}$ be the subset of $\mathcal{U}_n$, consisting of graphs whose (unique) cycle is of size k.

Proposition 6. *If $G \in \mathcal{U}_{n,k}$, then $\rho(G)$ depends only on the parameters n and k. For fixed n, $\rho(G)$ is a monotonically increasing function of k.*

Proposition 7. *If $G \in \mathcal{U}_n$, then $\rho(G)$ is maximal if and only if $G \cong C_n$.*

Proposition 8. *If $G \in \mathcal{U}_n k$, then $\rho(G)$ is minimal if and only if $pr^*(G) \cong C_3$.*

3.2 Bicyclic graphs

There are three types of bicyclic graphs without pendent vertices, depicted in Fig. 2.

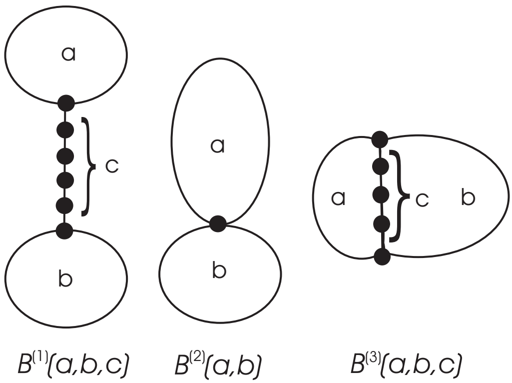

Fig. 2. Types of bicyclic graphs.

Note that $B^{(1)}(a,b,c)$ possesses $a+b+c$ vertices, $B^{(2)}(a,b)$ possesses $a+b-1$ vertices, and $B^{(3)}(a,b,c)$ possesses $a+b-c-2$ vertices, and that $a, b \geq 3$, $c \geq 0$.

For $i = 1,2,3$, denote by $\mathcal{B}^{(i)}$ the set of all connected bicyclic graph without pendent vertices, of type $B^{(i)}$.

Denote by $\mathcal{B}_n$ the set of connected bicyclic graphs with n vertices.

Proposition 9. *If $G \in \mathcal{B}_n$, then $\rho(G)$ is maximal if and only if $G \in \mathcal{B}^{(3)}$ for $n = a+b-c-2$, $a, b \geq 3$, $c \geq 0$.*

Proposition 10. *If $G \in \mathcal{B}_n$, then $\rho(G)$ is minimal if and only if $pr^*(G) \cong B^{(2)}(3,3)$.*

4 Path energy of graphs

The ordinary energy, $E(G)$, of a graph G is defined to be the sum of the absolute values of the ordinary eigenvalues of G [14]. In analogy, the *path energy*, $PE(G)$ is defined as the sum of the absolute values of the path eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of G, i.e.,

$$PE = PE(G) = \sum_{i=1}^{n} |\lambda_i| \,. \tag{2}$$

Some graphs have a single positive path eigenvalue (cf. Examples 1, 2, 4, and 5). For such graphs, since the sum of all path eigenvalues is equal to zero, $PE(G) = 2\,\rho(G)$.

If $\mathbf{P}(G)$ has several positive eigenvalues, then $PE(G) > 2\,\rho(G)$. However, if the greatest positive eigenvalue is much larger that the other positive eigenvalues, then as a reasonably accurate approximation, we have $PE(G) \approx 2\,\rho(G)$. As an example of this kind may serve the graph G depicted in Fig. 1, for which $\lambda_1 = 9.1$, $\lambda_2 = 0.7$ and λ_i is negative–valued for $i \geq 3$.

Bearing the above in mind, we may re-state the result of Corollary 1 as:

Conjecture 1. *Let G be a connected graph of order n.*
(i) $PE(G) \geq 2(n-1)$, with equality if and only if G is a tree of order n.
(ii) $PE(G) \leq 2(n-1)^2$, with equality if and only if $G \cong K_n$.

Results that would parallel Propositions 6–10 are the following:

Conjecture 2. *If $G \in \mathcal{U}_{n,k}$, then $PE(G)$ depends only on the parameters n and k. For fixed n, $PE(G)$ is a monotonically increasing function of k.*

Conjecture 3. *If $G \in \mathcal{U}_n$, then $PE(G)$ is maximal if and only if $G \cong C_n$.*

Conjecture 4. *If $G \in \mathcal{U}_n$, then $PE(G)$ is minimal if and only if $pr^*(G) \cong C_3$.*

Conjecture 5. *If $G \in \mathcal{B}_n$, then $PE(G)$ is maximal if and only if $G \in \mathcal{B}^{(3)}$ for $n = a+b-c-2$, $a, b \geq 3$, $c \geq 0$.*

Conjecture 6. *If $G \in \mathcal{B}_n$, then $PE(G)$ is minimal if and only if $pr^*(G) \cong B^{(2)}(3,3)$.*

Following an idea of Bapat and Pati [3,17], we characterize some properties of integer path energy.

Proposition 11. *Any even positive integer is the path energy of some graph.*

Proof. Let $m = 2k$ be a even positive integer. Consider a tree T with $k+1$ vertices. Then according to Example 1 and Eq. (2), $PE(T) = 2k = m$. ■

Proposition 12. *If the path energy $PE(G)$ of G is a rational number, then it is an even integer.*

Proof. We show that the claim of Proposition 12 holds for any symmetric square matrix whose elements are non-negative integers and whose diagonal is zero. Let $\mathbf{M}$ be such a matrix and let $\mu_1, \mu_2, \ldots, \mu_n$ be its eigenvalues. These eigenvalues are real–valued numbers.

The energy of $\mathbf{M}$ is

$$E(\mathbf{M}) = \sum_{i=1}^{n} |\mu_i| \, .$$

Let the positive eigenvalues of $\mathbf{M}$ be $\mu_1, \ldots, \mu_r$. Since $\sum_{i=1}^{n} \mu_i = 0$, it is easy to see that

$$E(\mathbf{M}) = 2\sum_{i=1}^{r} \mu_i \, . \tag{3}$$

Consider the Cartesian product $\mathbf{M}\oplus\mathbf{M}$ of the matrix $\mathbf{M}$ with itself [6,13,15], and recall that its eigenvalues are $\mu_i + \mu_j \ , \ i,j = 1,2,\ldots,n$. Therefore, the sum $\mu_1 + \mu_2 + \cdots + \mu_r$ is an eigenvalue of the r-fold Cartesian product $\mathbf{M} \oplus \mathbf{M} \oplus \cdots \oplus \mathbf{M}$.

The product $\mathbf{M} \oplus \mathbf{M} \oplus \cdots \oplus \mathbf{M}$ is also a symmetric square matrix whose elements are non-negative integers and whose diagonal is zero. Its characteristic polynomial is a monic polynomial with integer coefficients, and therefore any rational root of such a polynomial must be an integer. Thus, if $\mu_1 + \mu_2 + \cdots + \mu_r$ is a rational number, then it must be an integer. Then by Eq. (3), $E(\mathbf{M})$ must be an even integer. ■

5 Concluding remarks

After establishing the basic properties of the path matrix and its eigenvalues, it is necessary to address the question which structural property of the underlying graph is reflected by this matrix and its eigenvalues.

Bearing in mind Example 1, it is evident that $\mathbf{P}(G)$ and its eigenvalues are fully insensitive to any acyclic structural feature of the graph G. On the other hand, the presence, size, and mutual constellation of the cycles contained in G do affect the properties of $\mathbf{P}(G)$. This is, perhaps, best seen from Proposition 6, by means of which we may deduce the size of the cycle of a unicyclic graph – and nothing more.

Some time ago, a concept named *cyclicity* was put forward in mathematical chemistry [5], see also [18]. Analogous ideas are sporadically encountered also in graph theory [9,11]. Although there exists no precise definition of what cyclicity of a molecular graph might be, we may guess that the path matrix, its eigenvalues, and the path energy in particular, provide measures of molecular cyclicity. If this is of any practical value and applicability remains to be verified or disputed in the future.

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