Path matrix and path energy of graphs

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Abstract

Given a graph $G$, we associate a path matrix $P$ whose $(i, j)$ entry represents the maximum number of vertex disjoint paths between the vertices $i$ and $j$, with zeros on the main diagonal. In this note, we resolve four conjectures from [M. M. Shikare, P. P. Mal vadkar, S. C. Patekar, I. Gutman, On Path Eigenvalues and Path Energy of Graphs, MATCH Commun. Math. Comput. Chem. 79 (2018), 387–398.] on the path energy of graphs and finally present efficient $O(|E||V|^3)$ algorithm for computing the path matrix used for verifying computational results.

1 Introduction

Let $G$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Define the matrix $P = (p_{ij})$ of size $n \times n$ such that $p_{ij}$ is equal to the maximum number of vertex disjoint paths from $v_i$ to $v_j$ for $i \neq j$, and $p_{ij} = 0$ if $i = j$. We say that $P = P(G)$ is the path matrix of the graph $G$ [16]. $P$ is a real and symmetric matrix and therefore has real spectra $Spec_P$.

A path spectral radius of graph is largest eigenvalue $\rho = \rho(G)$ of the path matrix $P(G)$. Denote by $\deg(v)$ the degree of the vertex $v$, and with $\Delta(G)$ the largest vertex degree. The ordinary energy $E(G)$, of a graph $G$ is defined to be the sum of the absolute values of the ordinary eigenvalues of
In analogy, the path energy $PE(G)$ is defined as

$$PE(G) = \sum_{i=1}^{n} |\rho_i|.$$ 

Shikare et al. [5] studied basic properties of the path matrix and its eigenvalues. Here we continue the study by focusing on the extremal problems of path energy of graphs, and resolve open problems around the structure of general and unicyclic graphs attaining maximal or minimal values of $PE(G)$.

## 2 Extremal values of path energy of graphs

The authors in [5] proved the following two simple results

**Theorem 2.1** Let $G$ be a connected graph of order $n$. Then

(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 $G$ is a complete graph $K_n$.

**Theorem 2.2** Let $G$ be a graph with vertex set $V(G)$. Then for all $u, v \in V$, it holds

$$p_{uv}(G) \leq \min\{\deg(u), \deg(v)\}.$$ 

The following result resolves Conjecture 1 from [5].

**Theorem 2.3** Let $G$ be a connected graph of order $n$. Then

(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 $G$ is a complete graph $K_n$.

**Proof.** The trace of the matrix $P$ is 0 by definition, which is in turn the sum of all its eigenvalues. The first part directly follows from Theorem 2.1

$$PE(G) \geq 2\rho(G) \geq 2(n-1).$$

For the second part we use Cauchy-Schwarz inequality:

$$PE(G) = \rho(G) + \sum_{i=2}^{n} \rho_i(G) \leq \rho(G) + \sqrt{(n-1) \left( \sum_{i=2}^{n} \rho_i^2 \right)}.$$
Using Theorem 2.2, the trace of the squared matrix is clearly less than or equal to
\[ \text{Tr}(P^2) = \sum_{i=1}^{n} \rho_i^2 \leq n(n-1) \cdot \Delta^2 \leq (n-1)^4 n. \]

Combining the above, we get
\[ PE(G) \leq \rho + \sqrt{(n-1)^4 n - \rho^2(n-1)}. \]

The function \( f(x) = x + \sqrt{(n-1)^4 n - x^2(n-1)} \) is increasing for \( x \leq (n-1)^2 \), as the first derivative is non-negative:
\[ f'(x) = 1 - \frac{x(n-1)}{\sqrt{(n-1)^4 n - x^2(n-1)}} \geq 0, \]
which is equivalent with \((n-1)^4 n - x^2(n-1) \geq x^2(n-1)^2\).

The equality holds in both cases if and only if \( \rho \) attains minimum or maximum values, which follows from Theorem 2.1.

\[ \blacksquare \]

3 Path energy of unicyclic graphs

Let \( U_{n,k} \) be a unicyclic graph of the order \( n \) whose cycle is of the size \( k \).

In the following we give the results that resolves Conjectures 2, 3 and 4 from [5].

**Conjecture 3.1** Let \( G \) be a unicyclic graph of the order \( n \) whose cycle is of the size \( k \), then \( PE(G) \) depends only on the parameters \( n \) and \( k \). For fixed value of \( n \), \( PE(G) \) is a monotonically increasing function of \( k \).

First we determine the spectrum of the path matrix of unicyclic graphs. If \( k = n \), that is \( U_{n,k} \cong C_n \), it is easy to see that \( P(U_{n,k}) = 2J_n \), where \( J_n \) is the square matrices of the order \( n \) whose all non-diagonal elements are equal to one, and all diagonal elements are zero. Furthermore, as \( J_n \) represents the adjacency matrix of the complete graph \( K_n \) we obtain that
\[ \text{Spec} P(C_n) = \left( (-2)^{n-1}, 2(n-1)^1 \right). \]

Next we calculate the spectrum of \( P(U_{n,k}) \) for \( k \leq n-1 \).
Theorem 3.2 The spectrum of the path matrix of the unicyclic graph $U_{n,k}$, for $k \leq n - 1$, is equal to

$$\text{Spec}(U_{n,k}) = \left( (-2)^{k-1} (-1)^{n-k-1} \rho_2 \rho_1 \right),$$

where

$$\rho_{1,2} = \frac{n + k - 3 \pm \sqrt{(n + k - 3)^2 + 4(k^2 - nk + 2n - 2)}}{2}. \tag{1}$$

Proof. The vertices of $U_{n,k}$ can be labeled so that

$$P(U_{n,k}) = \left[ \begin{array}{c|c} P(C_k) & 1 \\ \hline 1 & J_{n-k} \end{array} \right] = \left[ \begin{array}{c|c} 2J_k & 1 \\ \hline 1 & J_{n-k} \end{array} \right].$$

Now, we will determine the roots of the characteristic polynomial

$$\det(P(U_{n,k}) - \lambda I_n) = \begin{vmatrix} 2J_k - \lambda I_k & 1 \\ 1 & J_{n-k} - \lambda I_{n-k} \end{vmatrix},$$

where $I_s$ is identity matrix of the order $s$. By subtracting the $s$-th row from the $(s-1)$-th row, for $2 \leq s \leq k$, and by subtracting the $s$-th row from the $(s+1)$-th row, for $k+1 \leq s \leq n - 1$, we obtain that the $s$-th row is equal to

$$[0, \ldots, 0, \lambda + 2, -\lambda - 2, 0, \ldots, 0]$$

for $2 \leq s \leq k$, and the $l$-th row is equal to

$$[0, \ldots, 0, -\lambda - 1, \lambda + 1, 0, \ldots, 0]$$

for $k + 1 \leq l \leq n - 1$. Therefore, we conclude that

$$(\lambda + 2)^{k-1}(\lambda + 1)^{n-k-1} \mid \det(P(U_{n,k}) - \lambda I_n)$$

and hence it is proved that $P(U_{n,k})$ has the eigenvalues $-2$ and $-1$ with multiplicities $k - 1$ and $n - k - 1$, respectively. Notice that $n - k - 1 \geq 0$, as $k - 1 \leq n$.

Now, we will determine the other two eigenvalues. As the trace of $P(U_{n,k})$ is equal to zero and the trace of $P(U_{n,k})^2$ is equal to the sum of the squares of the entries of $P(U_{n,k})$ we have that

$$\sum_{i=1}^{n} \rho_i = \text{tr}(P(U_{n,k})) = 0$$

$$\sum_{i=1}^{n} \rho_i^2 = \text{tr}(P(U_{n,k})^2) = 4(k^2 - k) + (n^2 - k^2 - (n - k)).$$
Furthermore, since we have already concluded that 
\[ (\rho_3, \ldots, \rho_n) = \left( \frac{-2, \ldots, -2, -1, \ldots, -1}{k-1} \right)_{n-k-1} \]
it holds that
\[ \rho_1 + \rho_2 = 2(k - 1) + (n - k - 1) \quad (2) \]
\[ \rho_1^2 + \rho_2^2 = 4(k^2 - k) + (n^2 - k^2 - (n - k)) - 4(k - 1) - (n - k - 1). \quad (3) \]
By substituting the variable \( \rho_2 \) from first equation to the second, we get
\[ 2\rho_1^2 - 2(n + k - 2)\rho_1 - 2k^2 + 2nk - 4n + 4 = 0, \]
which completes the proof.

From the above theorem directly follows that
\[ \rho_1 = \frac{n + k - 3 + \sqrt{(n + k - 3)^2 + 4(k^2 - nk + 2n - 2)}}{2} \]
is the spectral radius of \( U_{n,k} \) for \( 3 \leq k \leq n - 1 \).

By analyzing the above formula we can obtain Propositions 6, 7 and 8 from [5]. Indeed, if we denote
\[ f(x) = n + x - 3 + \sqrt{(n + x - 3)^2 + 4(x^2 - nx + 2n - 2)} \]
then it is sufficient to prove that \( f(x) \) is monotonically increasing function of \( x \), for \( 2 \leq x \leq n - 1 \), to get Proposition 6. First derivative of \( f(x) \) is equal to \( 1 + \frac{5x - n - 3}{\sqrt{D(x)}} \), where \( D(x) = (n + x - 3)^2 + 4(x^2 - nx + 2n - 2) \). If \( x \geq \frac{n+3}{5} \) then it is clear that \( f'(x) \geq 0 \). Now, for \( 1 \leq x < \frac{n+3}{5} \) we prove that \( \sqrt{D(x)} > n + 3 - 5x \). After a short calculation, it can be obtained that \( D(x)^{2} > (5x - n - 3)^{2} \) if and only if \( 5x^2 - 2(n + 3)x + n + 2 < 0 \). Since this quadratic function is convex, it is less than zero in the interval \( (x_1, x_2) \), where \( x_{1,2} = \frac{n+3 \pm \sqrt{(n+3)^2 - 5(n+2)}}{5} \). It is easy to check that \( x_2 \leq 1 \) and \( x_1 \geq \frac{n+3}{5} \) and therefore we conclude \( \sqrt{D(x)} > n + 3 - 5x \) and \( f'(x) > 0 \) for \( 1 \leq x < \frac{n+3}{5} \).

From \( \frac{f(n-1)}{2} < 2(n-1) \) if and only if \( n > 1 \) follows Proposition 7. Finally, we can calculate minimal spectral radius in the class of unicyclic graphs of the order \( n \) and it is attained for \( k = 3 \):
\[ \min_{3 \leq k \leq n} \rho(U_{n,k}) = \frac{f(3)}{2} = \frac{n + \sqrt{n^2 - 4n + 28}}{2}. \]
Lemma 3.3 The eigenvalue $\rho_2$ of the path matrix of the unicyclic graph $U_{n,k}$, for $k \leq n - 1$, is greater to zero if and only if $n \geq 7$ and $3 \leq k \leq n - 3$.

Proof. According to (1) we conclude that $\rho_2 > 0$ if and only if $k^2 - nk + 2n - 2 < 0$. If we denote $k^2 - nk + 2n - 2$ by $g(k)$, then we have that $g(k) < 0$ if and only if $k$ belongs to the interval $(x_1, x_2)$, where $x_{1,2} = \frac{n \pm \sqrt{n^2 - 8n + 8}}{2} \in \mathbb{R}$. Furthermore, $x_{1,2} \in \mathbb{R}$ if and only if $n^2 - 8n + 8 \geq 0$ and this is the case for $(n - 4)^2 - 8 \geq 0 \iff n \geq 4 + \sqrt{8}$. Therefore, $x_{1,2} \in \mathbb{R}$ if and only if $n \geq 7$.

On the other hand, we may notice that $x_2 = n - 4 - \sqrt{(n - 4)^2 - 8} + 2 > 2$ and $x_2 = n - 6 - \sqrt{(n - 6)^2 + (4n - 28)} + 3 \leq 3$,
as $4n - 28 \geq 0$. From Vieta’s formulas we have that $x_1 + x_2 = n$ and therefore $n - 3 < x_2 \leq n - 2$. Finally, since $k$ is integer we conclude that $3 = \lfloor x_2 \rfloor + 1 \leq k \leq \lfloor x_2 \rfloor = n - 3$. □

Now, we calculate the path energy of unicyclic graph of the order $n$ and cycle length $k$, such that $k \leq n - 1$. According to the previous lemma the spectrum of $U_{n,k}$ has two positive eigenvalues $\rho_1$ and $\rho_2$ if and only if $n \geq 7$ and $3 \leq k \leq n - 3$. In that case, the energy of $U_{n,k}$ is equal to $2(\rho_1 + \rho_2)$ and from (2) we further have that it is equal to $2(n + k - 3)$. Now, if $n < 7$ or $n - 2 \leq k \leq n - 1$ then we conclude that $\rho_1$ is the only positive eigenvalue-spectral radius and the path energy is equal to $2\rho_1$.

Theorem 3.4 The path energy of unicyclic graph $U_{n,k}$ for $3 \leq k \leq n - 1$, is equal to

$$PE(U_{n,k}) = \begin{cases} 2(n + k - 3), & n \geq 7 \text{ and } 3 \leq k \leq n - 3 \\ 2\rho(U_{n,k}), & n < 7 \text{ or } n - 2 \leq k \leq n - 1 \end{cases}$$

where $\rho(U_{n,k}) = \rho_1 = \frac{n + k - 3 + \sqrt{(n + k - 3)^2 + 4(k^2 - nk + 2n - 2)}}{2}$ is the spectral radius of $U_{n,k}$.

Since it has already shown that $\rho(U_{n,k})$ is increasing function of $k$, and as $2(n + k - 3)$ is increasing as well, it remains to prove that

$$2(n + (n - 3) - 3) < 2\rho(U_{n,n-2}).$$
Indeed, as $2\rho(U_{n,k}) = n + k - 3 + \sqrt{(n+k-3)^2 + 4g(k)}$, where $g(k) = k^2 - nk + 2n - 2$, we conclude that

$$2\rho(U_{n,k}) > n + k - 3 + \sqrt{(n+k-3)^2 + 0} = 2(n+k-3) > 2(n+(n-3)-3),$$

for $n - 2 \leq k \leq n - 1$ (in the proof of Lemma 3.3 we have used that $g(k) < 0$ if and only if $3 \leq k \leq n - 3$). Therefore, we see that $PE(U_{n,k})$ is increasing function of $k$ and hence we prove Conjecture 3.1 from [5].

Conjecture 3 and 4 can be unified and generalized in the following way:

**Theorem 3.5** Let $G$ be an unicyclic graph of order $n$. Then

(i) $PE(G) \leq 4(n - 1)$ with equality if and only if $G \cong C_n$,

(ii) $PE(G) \geq n + \sqrt{n^2 - 4n + 28}$ with equality if and only if $G \cong U_{n,3}$.

**Proof.** From the above discussion implies that $PE(U_{n,k})$, for $3 \leq k \leq n - 1$, is maximal for $k = n - 1$. Since $PE(C_n) = 4(n - 1)$ it remains to compare the values $PE(U_{n,n-1})$ and $PE(C_n)$. It can be directly verified that the inequality

$$PE(U_{n,n-1}) = 2n - 4 + \sqrt{(2n - 4)^2 + 4((n-1)^2 - n(n-1) + 2n - 2)} \leq 4(n-1)$$

holds if and only if $n \geq 3$.

Moreover, the minimal path energy in the class of unicyclic graphs of the order $n$ is attained for $k = 3$:

$$\min_{3 \leq k \leq n} PE(U_{n,k}) = n + \sqrt{n^2 - 4n + 28}.$$

■

4 Efficient algorithm for computing the matrix $P(G)$

In order to find the maximum number of vertex disjoint paths between two vertices, we can transform it to the problem of finding maximum number of edge disjoint paths. For all vertices except fixed vertices $x$ and $y$, split vertex $v$ into $v_{in}$ and $v_{out}$ with an edge $v_{in} \rightarrow v_{out}$. If we had an edge $uv$ in the original graph, this gets converted to two directed edges $u_{out} \rightarrow v_{in}$ and $v_{out} \rightarrow u_{in}$.

Using Max-Flow Min-Cut theorem, the problem is now equivalent to computing maximum flow for any two pairs of vertices. We can use Ford-Fulkerson algorithm [2] for computing maximum flow in $O(|E| \cdot \max |F|) = $
we have all edge capacities equal to 1 in the graph $G$. For all pairs of vertices this gives us an algorithm of complexity $O(|E||V|^3)$.

A biconnected graph is a connected and non-separable graph, meaning that if any one vertex were to be removed, the graph will remain connected. The running time can be further speed up by finding all articulation points and biconnected components in time $O(|E|+|V|)$ as only within biconnected components the values of the matrix $P$ can be larger than 1. This can be done in a preprocessing step.

We plan to use this efficient algorithm to continue studying the path energy of graphs, in particular bicyclic and biconnected graphs.

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