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On the extensional eigenvalues of graphs

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A B S T R A C T

Assume that G is a graph on n vertices with associated symmetric matrix M and K a positive definite symmetric matrix of order n. If there exists $0 \neq x \in \mathbb{R}^n$ such that $Mx = \lambda Kx$, then λ is called an extensional eigenvalue of G with respect to K. This concept generalizes some classic graph eigenvalue problems of certain matrices such as the adjacency matrix, the Laplacian matrix, the diffusion matrix, and so on. In this paper, we study the extensional eigenvalues of graphs. We develop some basic theories about extensional eigenvalues and present some connections between extensional eigenvalues and the structure of graphs.

1. Introduction

Throughout this paper, we only consider undirected graphs without loops or parallel edges and their associate matrices in $\mathbb{R}^{n\times n}$. Assume that $G = (V, E)$ is a graph where V is the vertex set and E is the edge set. For two vertices $u, v \in V$, the *distance* $d_G(u, v)$ of them is the length of a shortest path from u to v. For $v \in V(G)$ and $i \geq 0$, the *i-neighborhood* of v is $N_G^{(i)}(v) = \{u \in V(G) : d(u, v) = i\}$. It is clear that $N_G^{(0)}(v) = \{v\}$ and $V(G) = \sum_{i\geq 0} N_G^{(i)}(v)$. The *neighborhood* $N_G(v)$ of v is just the 1-neighborhood of v, that is $N_G(v) = N_G^{(1)}(v)$. The *degree* of v, denoted by $d_G(v)$, is the cardinality of $N_G(v)$, that is, $d_G(v) = |N_G(v)|$. All other notions in graph theory are from [1].

For spectral graph theory, one is often interested in the following matrices.

- Degree matrix: $D(G)$ a diagonal matrix indexed by V whose vth diagonal entry is $d_G(v)$.
- Adjacency matrix: $A(G)$ a square matrix indexed by V whose (u, v)-entry is 1 if $uv \in E$ and 0 otherwise.
- Randic matrix: $R(G) = D(G)^{-1/2}A(G)D(G)^{-1/2}$.
- Diffusion matrix (also known as the transition probability matrix): $W(G) = D(G)^{-1}A(G)$ which is similar to $R(G)$.
- Laplacian matrix: $L(G) = D(G) - A(G)$.
- Signless Laplacian matrix: $Q(G) = D(G) + A(G)$.
- Normalized Laplacian matrix: $\mathcal{L}(G) = D(G)^{-1/2}L(G)D(G)^{-1/2}$.

If there is no confusion, usually we delete the symbol G is the notations such as $d_G(v)$, $N_G^{(i)}(v)$ and $A(G)$.

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Let $M \in \mathbb{R}^{n\times n}$ be a symmetric matrix associate to the graph G. If there exists $0 \neq x \in \mathbb{R}^n$ such that $Mx = \lambda x$, then λ is an *eigenvalue* of M with eigenvector x. Such eigenvalues are also called *M-eigenvalues* of G. The collection of all such eigenvalues is the *M-spectrum* of G, denoted by $Sp_M(G)$.

Let $\mathcal{P}(n)$ be the set of all positive definite symmetric matrices in $\mathbb{R}^{n\times n}$. For a matrix $K \in \mathcal{P}(n)$ and a symmetric matrix M associate to the graph G, if there exists $0 \neq x \in \mathbb{R}^n$ such that $Mx = \lambda Kx$, then λ is called an **extensional eigenvalue** of M with respect to K (or *(M,K)-eigenvalue* for short), and x is called the corresponding *(M,K)-eigenvector*. The multiset of all such eigenvalues is the *M-extensional spectrum* of G with respect to K (or *(M,K)-spectrum* for short), denoted by $Sp_M(G, K)$.

The (A, K)-eigenvalues are called the extensional eigenvalues of G and the (A, K)-spectrum is called the extensional spectrum of G, denoted by $\mathrm{Sp}(G, K)$. It is clear that $\mathrm{Sp}(G, I) = \mathrm{Sp}(G)$. Therefore, it is natural to ask whether the extensional spectrum of a graph possess the similar properties of adjacency spectrum. In general, the extensional spectral problems (also called the generalized spectral problems) mainly study the connections between the extensional spectra and the combinatorial structures of graphs. Note that the extensional eigenvalues of a graph are natural generalizations of the above mentioned matrix eigenvalues if we take $K = I_n$, and has many applications in numerical computations, see, for example, Boutry et al. [2] and the references therein for more details. It would be interesting to consider this new generalization.

In this paper, we try to develop the basic theories on extensional eigenvalues of graphs. In Section 2, we present some basic properties about extensional spectra. In Section 3, we introduce the so called extensional Rayleigh quotient and investigate the extensional spectral radius. In Section 4, we investigate how that extensional spectrum of a graph reveals the structure properties of the graph. In Section 5, we leave some problems for further research.

2. Properties and results

Let G be a graph with associate symmetric matrix M and $K \in \mathcal{P}(n)$. Some basic properties of (M, K)-eigenvalues of G are investigated in this part. Since K is positive definite, from the Cholesky decomposition, there exists a non-singular matrix P such that $K = P^{\mathrm{T}}P$, and thus we have $Mx = \lambda P^{\mathrm{T}}Px$ or equally $((P^{-1})^{\mathrm{T}}MP^{-1})(Px) = \lambda(Px)$. By setting $S = (P^{-1})^{\mathrm{T}}MP^{-1}$ and $y = Px$, we have $Sy = \lambda y$. As S is also symmetric, its eigenvalues are real. Suppose all its eigenvalues are $\lambda_1, \lambda_2, \dots, \lambda_n$, then there is an orthogonal matrix U such that $U^{\mathrm{T}}SU = diag(\lambda_1, \lambda_2, \dots, \lambda_n)$. Assume that $U = (u_1, u_2, \dots, u_n)$. It follows that

$$Su_j = \lambda_j u_j, \quad \text{for } j = 1, 2, \dots, n.$$

As U is orthogonal, $u_1, u_2, \dots, u_n$ are mutually orthogonal unit eigenvector of S. Denote by $q_j = P^{-1}u_j$ for $1 \le j \le n$, then we have

$$Mq_j = (P^{\mathrm{T}}SP)(P^{-1}u_j) = P^{\mathrm{T}}Su_j = P^{\mathrm{T}}(\lambda_j u_j) = \lambda_j P^{\mathrm{T}}u_j = \lambda_j (P^{\mathrm{T}}P)P^{-1}u_j = \lambda_j Kq_j.$$

This implies that λ_j for $1 \le j \le n$ are the extensional eigenvalues of M corresponding to K. Note that

$$q_i^{\mathrm{T}}Kq_j = q_i^{\mathrm{T}}(P^{\mathrm{T}}P)q_j = (Pq_i)^{\mathrm{T}}(Pq_j) = u_i^{\mathrm{T}}u_j = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$$

We conclude that $q_1, q_2, \dots, q_n$ are linear independent. In fact, if $a_1q_1 + a_2q_2 + \ldots + a_nq_n = 0$ then $q_i^{\mathrm{T}}K(a_1q_1 + a_2q_2 + \ldots + a_nq_n) = 0$ for any i. It leads to $a_i = 0$ for $1 \le i \le n$. In general, for a matrix $K \in \mathcal{P}(n)$ and verctors $v_1, v_2, \dots, v_n \in \mathbb{R}^n$, we say that $v_1, v_2, \dots, v_n$ are *K-orthogonal* if $v_i^{\mathrm{T}}Kv_j = 0$ for any $i \neq j$. If, additional, $v_i^{\mathrm{T}}Kv_i = 1$ for any i then these vectors are called *K-orthonormal*. Therefore, the vectors q_i for $1 \le i \le n$ are K-orthonormal (M, K)-eigenvectors.

Note that the adjacency eigenvalues of a graph are all real and there exist eigenvectors which form a basis of $\mathbb{R}^n$. We get the similar results for the extensional eigenvalues by the arguments above.

Remark 1. Let G be a graph on n vertices with associated real symmetric matrices M and $K \in \mathcal{P}(n)$. Then we have

(i) all (M, K)-eigenvalues are real, and thus can be listed as $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_n$;
(ii) there exist (M, K)-orthonormal eigenvectors $q_1, q_2, \dots, q_n$ which form a basis of $\mathbb{R}^n$.

The following properties are immediate from the definition of extensional eigenvalues.

Property 1. *If the* matrix M *is positive semi-definite, then all* (M, K)*-eigenvalues of* G *are non-negative.*

Property 2. *If the matrix* M *is singular, then 0 is an* (M, K)*-eigenvalue of* G*.*

Proof. Note that $S = (P^{-1})^{\mathrm{T}}MP^{-1}$ is also sigular as M is singular, where P is the non-sigular matrix defined above satisfying $K = P^{\mathrm{T}}P$. By noticing that the (M, K)-eigenvalues are just the eigenvalues of S, the result follows. □

Property 3. *If* G *has a partition* $V(G) = V_1 \cup V_2$ *such that* $M[V_1, V_1] = 0$, $M[V_2, V_2] = 0$ *and* $K[V_1, V_2] = 0$, *then the* (M, K)*-eigenvalues of* G *are symmetric about 0.*

Remark 2. This property indicates that the eigenvalues (i.e., (A, I)-eigenvalues) of a bipartite graph are symmetric about 0.

To end this part, we give some examples of the extensional eigenvalues for the different choices of M and K.

- If we take $M = A(G)$ and $K = I_n$, then the extensional eigenvalue problem for graphs becomes the ordinary eigenvalue problem.
- If we take $M = A(G), K = D(G)$, then the $(A(G), D(G))$-eigenvalues are just the eigenvalues of $W(G) = D(G)^{-1}A(G)$. Suppose such eigenvalues are $1 = \mu_1 \geq \mu_2 \geq \ldots \mu_n \geq -1$ (they also are the eigenvalues of $R(G)$), as suggested in Chung [3]. It is known that $\mu_1 = 1$ if and only if G is a non-trivial bipartite graph.
- If we take $M = D(G) - A(G), K = D(G)$, then $(D(G) - A(G))x = \lambda D(G)x$ implies that $A(G)x = (1-\lambda)D(G)x$. It follows that $1 - \lambda = \mu_i$ and therefore $\lambda = 1 - \mu_i$ for $i = 1, 2, \ldots, n$. These are the eigenvalues of the normalized Laplacian matrix $\mathcal{L}(G)$ of G in light of Chapter 1 in Chung [3].
- If we take $M = A(G), K = Q(G) = D(G) + A(G)$, then for a non-bipartite connected graph G, $Q(G)$ is positive definite. Suppose $A(G)x = \lambda(D(G) + A(G))x$ with $x \neq 0$, then we have $(1-\lambda)A(G)x = \lambda D(G)x$ and $\lambda \neq 1$. Hence it follows that $\frac{\lambda}{1-\lambda} = \mu_i$ and therefore $\frac{\mu_i}{1+\mu_i} = \lambda$ for $i = 1, 2, \ldots, n$.
- If we take $M = D(G) - A(G), K = Q(G) = D(G) + A(G)$, then for a non-bipartite connected graph G, $Q(G)$ is positive definite. Suppose $(D(G) - A(G))x = \lambda(D(G) + A(G))x$ with $x \neq 0$, then we have $(1+\lambda)A(G)x = (1-\lambda)D(G)x$ and $\lambda \neq -1$. Hence it follows that $\frac{1-\lambda}{1+\lambda} = \mu_i$ and therefore $\lambda = \frac{1-\mu_i}{1+\mu_i}$ for $1 \leq i \leq n$ are (M, K)-eigenvalues of G.
- If we take $M = \alpha D(G) + (1-\alpha)A(G)$ with $0 \leq \alpha \leq 1$, $K = D(G)$, then for a connected graph G, suppose $(\alpha D(G) + (1-\alpha)A(G))x = \lambda D(G)x$ with $x \neq 0$, then we have $\lambda = 1$ if $\alpha = 1$. If $\alpha \neq 1$, then $(1-\alpha)A(G)x = (\lambda - \alpha)D(G)x$. Hence it follows that $\frac{\lambda-\alpha}{1-\alpha} = \mu_i$ and therefore $\lambda = (1-\alpha)\mu_i + \alpha$ for $1 \leq i \leq n$ are (M, K)-eigenvalues of G.
- If we take $M = \alpha D(G) + (1-\alpha)A(G)$ with $0 \leq \alpha \leq 1$, $K = Q(G) = D(G) + A(G)$, then for a non-bipartite connected graph G, suppose $(\alpha D(G) + (1-\alpha)A(G))x = \lambda(D(G) + A(G))x$ with $x \neq 0$, then we have $\lambda = \frac{1}{2}$ if $\alpha = \frac{1}{2}$. If $\alpha \neq \frac{1}{2}$, then $(1-\alpha-\lambda)A(G)x = (\lambda - \alpha)D(G)x$ and $\lambda \neq 1 - \alpha$. Hence it follows that $\frac{\lambda-\alpha}{1-\alpha-\lambda} = \mu_i$ and therefore $\lambda = \frac{(1-\alpha)\mu_i+\alpha}{1+\mu_i}$ for $1 \leq i \leq n$ are (M, K)-eigenvalues of G.

From the above examples, we see that the extensional eigenvalue problems for graphs are closely related to many other graph matrices, and may be deduce new perspective.

3. The extensional Rayleigh quotient

In this part, we introduce the extensional Rayleigh quotient and investigate the extensional spectral radius of a graph.

Recall that, for $0 \neq x \in \mathbb{R}^n$ and the adjacency matrix A of a graph G, the form $\frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x}$ is called the *Rayleigh quotient* of A. By this notion, many interesting results were obtained, for example,

$$\lambda_1 = \max\left\{\frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x} : x \in \mathbb{R}^n \setminus \{0\}\right\} \text{ and } \lambda_i = \min\left\{\max\left\{\frac{x^{\mathrm{T}}Ax}{x^{\mathrm{T}}x} : x \in U \setminus \{0\}\right\} : U \in \mathcal{U}_{n-i+1}\right\},$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are the eigenvalues of A and $\mathcal{U}_{n-i+1}$ is the set of all $(n-i+1)$-dimensional subspaces of $\mathbb{R}^n$. Let $K \in \mathcal{P}(n)$ be a matrix, G a graph with associate real symmetric matrix M and $0 \neq x \in \mathbb{R}^n$. The form $\frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx}$ is called the *Rayleigh quotient of M with respect to K*. In what follows, we obtain parallel results for extensional eigenvalues.

Theorem 1. *Let G be a graph on n vertices, $M \in \mathbb{R}^{n\times n}$ an associate symmatrix and $P \in \mathcal{P}(n)$. If $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are (M, K)-eigenvalues of G, then*

$$\lambda_i = \min_{U \in \mathcal{U}_{n-i+1}} \max\left\{\frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx} : x \in U\right\}$$

where $\mathcal{U}_{n-i+1}$ is the set of all $(n-i+1)$-dimensional subspaces of $\mathbb{R}^n$.

Proof. Assume that $K = P^{\mathrm{T}}P$ is the Cholesky decomposition of K. Let $y_1, y_2, \ldots, y_n$ be the orthonormal eigenvectors of $S = (P^{-1})^{\mathrm{T}}MP^{-1}$ and $x_i = P^{-1}y_i$ for $1 \leq i \leq n$. According to Remark 1 (ii), $x_1, \ldots, x_n$ are K-orthonormal (M, K)-eigenvectors and form a basis of $\mathbb{R}^n$. Therefore, for any $0 \neq x \in \mathbb{R}^n$, there exist $a_1, a_2, \ldots, a_n \in \mathbb{R}$ such that $x = \sum_{i=1}^n a_i x_i$, and thus

$$\frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx} = \frac{(\sum_{k=1}^n a_k x_k)^{\mathrm{T}} M (\sum_{k=1}^n a_k x_k)}{(\sum_{k=1}^n a_k x_k)^{\mathrm{T}} K (\sum_{k=1}^n a_k x_k)} = \frac{\sum_{k=1}^n a_k^2 \lambda_k}{\sum_{k=1}^n a_k^2}. \tag{1}$$

For any $U \in \mathcal{U}_{n-i+1}$, it is clear that $\dim U \cap \langle x_1, x_2, \ldots, x_i\rangle \geq 1$. Taking $x \in U \cap \langle x_1, x_2, \ldots, x_i\rangle$, we have $a_j = 0$ for $j \geq i+1$. From (1), we have

$$\max\left\{\frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx} : x \in U\right\} \geq \frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx} = \frac{\sum_{k=1}^i a_k^2 \lambda_k}{\sum_{k=1}^i a_k^2} \geq \lambda_i.$$

Thus, $\lambda_i \leq \min_{U \in \mathcal{U}_{n-i+1}} \max\left\{\frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx} : x \in U\right\}$.

On the other hand, by taking $U_0 = \langle x_i, x_{i+1}, \ldots, x_n\rangle \in \mathcal{U}_{n-i+1}$, one can easily verify that $\max\left\{\frac{x^{\mathrm{T}}Mx}{x^{\mathrm{T}}Kx} : x \in U_0\right\} = \lambda_i^{(K)}$ according to (1). Thus the result follows. $\square$

From Theorem 2, one can get the following results immediately.

Corollary 1. *Let G be a graph with associate real symmetric matrix M and* $K \in \mathcal{P}(n)$*. If* $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ *are* (M, K)*-eigenvalues of G, then* $\lambda_1 = \max_{x\neq 0} \frac{x^T Mx}{x^T Kx}$ *and* $\lambda_n^{(K)} = \min_{x\neq 0} \frac{x^T Mx}{x^T Kx}$.

From Corollary 1, taking x being the all one vector, we have

Corollary 2. *Let G be a graph with associate real symmetric matrix* $M = (m_{ij})$ *and* $K = (k_{ij}) \in \mathcal{P}(n)$*. If* $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ *are* (M, K)*-eigenvalues of G, then*

$$\lambda_1 \geq \frac{\sum_{i,j=1}^n m_{i,j}}{\sum_{i,j=1}^n k_{i,j}} \geq \lambda_n.$$

We call the maximum absolute value of the (M, K)-eigenvalues the *extensional spectral radius*, and denoted by $\rho(M, K)$, that is, $\rho(M, K) = \max\{|\lambda_i| : i = 1, 2, \ldots, n\}$. Obviously, $\rho(M, K) = \max\{|\lambda_1|, |\lambda_n|\}$.

From the above, we deduce some interesting results in the following.

Theorem 2. *Let M be a real symmetrix matrix and* $K \in \mathcal{P}(n)$*. Then* $\rho(M, K) \leq 1$ *if and only if* $|x^T Mx| \leq x^T Kx$ *for any* $x \neq 0$.

Proof. Obviously,

$$\rho(M, K) = \max\left\{\left|\max_{x\neq 0} \frac{x^T Mx}{x^T Kx}\right|, \left|\min_{x\neq 0} \frac{x^T Mx}{x^T Kx}\right|\right\} = \max_{x\neq 0} \frac{|x^T Mx|}{x^T Kx}.$$

Thus $\rho(M, K) \leq 1$ if and only if $\frac{|x^T Mx|}{x^T Kx} \leq 1$ for any $x \neq 0$, which implies the result. □

Remark 3. By noticing that

$$|x^T A(G)x| = \left|2\sum_{uv\in E} x_u x_v\right| \leq \sum_{uv\in E} 2|x_u||x_v| \leq \sum_{uv\in E}(x_u^2 + x_v^2) = \sum_{v\in V} d(v)x_v^2 = x^T D(G)x,$$

we have $\rho(A(G), D(G)) \leq 1$ according to Theorem 2. Note that the $(A(G), D(G))$-eigenvalues are just the eigenvalues of the Randic matrix $R(G)$. Theorem 2 also indicates that the spectral radius of $R(G)$ is not greater than 1.

Theorem 3. *Let M be a positive semidefinite symmetric matrix and* $K \in \mathcal{P}(n)$*. Suppose* $\tau_i(T)$ *is the ith largest eigenvalue of a matrix T. Then we have*

$$\tau_1(KM) \leq \tau_1(K)\tau_1(M) \quad \text{and} \quad \tau_n(KM) \geq \tau_n(K)\tau_n(M).$$

Proof. We just prove the first one, the second follows similarly.

Since $(KM)x = \tau x$ is equivalent to $Mx = \tau K^{-1}x$, therefore the eigenvalues of KM is the extensional eigenvalues of M with respect to K^{-1}. So we have

$$\begin{aligned}
\tau_1(KM) &= \max_{x\neq 0} \frac{x^T Mx}{x^T K^{-1}x} = \max_{x\neq 0}\left(\frac{x^T Mx}{x^T x} / \frac{x^T K^{-1}x}{x^T x}\right) \\
&\leq \left(\max_{x\neq 0} \frac{x^T Mx}{x^T x}\right) / \left(\min_{x\neq 0} \frac{x^T K^{-1}x}{x^T x}\right) \\
&= \frac{\tau_1(M)}{\tau_n(K^{-1})} = \tau_1(K)\tau_1(M).
\end{aligned}$$

□

4. Eigenvalues and structures

In this part, we investigate the relationship between the extensional eigenvalues and the structure of a graph. We start at the result similar to the famous Perron Frobenius theorem. The following result follows from [4].

Theorem 4. *Let* $K \in \mathbb{R}^{n\times n}$ *be a positive definite matrix with all off-diagonal elements being non-positive. Then all entries of* K^{-1} *are non-negative.*

Proof. By induction on n. For $n = 1$, the result is obvious. Now we suppose the result holds for $n - 1$ and consider the case of n. We now write K as

$$K = \begin{bmatrix} K_1 & \alpha \\ \beta^T & a_{nn} \end{bmatrix},$$

where $\alpha, \beta \in \mathbb{R}^{(n-1)\times 1}$ and $K_1 \in \mathbb{R}^{(n-1)\times(n-1)}$. Since K is positive definite, we have $\det(K_1) > 0$. Therefore, we have

$$\begin{bmatrix} I_{(n-1)} & 0 \\ -\beta^T K_1^{-1} & 1 \end{bmatrix}\begin{bmatrix} K_1 & \alpha \\ \beta^T & a_{nn} \end{bmatrix}\begin{bmatrix} I_{(n-1)} & -K_1^{-1}\alpha \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} K_1 & 0 \\ 0 & a_{nn} - \beta^T K_1^{-1}\alpha \end{bmatrix}.$$

Taking determinant in both sides, we get $\det(K) = (a_{nn} - \beta^{\mathrm{T}} K_1^{-1} \alpha)\det(K_1)$. As $\det(K_1) > 0$ and $\det(K) > 0$, we have $a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha > 0$. Note that

$$K = \begin{bmatrix} K_1 & \alpha \\ \beta^{\mathrm{T}} & a_{nn} \end{bmatrix} = \begin{bmatrix} I_{(n-1)} & 0 \\ \beta^{\mathrm{T}} K_1^{-1} & 1 \end{bmatrix} \begin{bmatrix} K_1 & 0 \\ 0 & a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha \end{bmatrix} \begin{bmatrix} I_{(n-1)} & K_1^{-1}\alpha \\ 0 & 1 \end{bmatrix}.$$

We have

$$K^{-1} = \begin{bmatrix} K_1 & \alpha \\ \beta^{\mathrm{T}} & a_{nn} \end{bmatrix}^{-1} = \begin{bmatrix} I_{(n-1)} & -K_1^{-1}\alpha \\ 0 & 1 \end{bmatrix} \begin{bmatrix} K_1^{-1} & 0 \\ 0 & (a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1} \end{bmatrix} \begin{bmatrix} I_{(n-1)} & 0 \\ -\beta^{\mathrm{T}} K_1^{-1} & 1 \end{bmatrix},$$

which is

$$\begin{bmatrix} K_1^{-1} + (a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1} K_1^{-1}\alpha\beta^{\mathrm{T}} K_1^{-1} & -(a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1} K_1^{-1}\alpha \\ -(a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1}\beta^{\mathrm{T}} K_1^{-1} & (a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1} \end{bmatrix}.$$

As $a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha > 0$, therefore the (n,n)th entry of K^{-1} is positive. By induction hypothesis, all entries of K_1^{-1} are non-negative, while all elements of β are non-positive, so $-(a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1}\beta^{\mathrm{T}} K_1^{-1}$ has non-negative elements, and so does $-(a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1} K_1^{-1}\alpha$. As $\alpha\beta^{\mathrm{T}}$ has non-negative elements, so we have $K_1^{-1} + (a_{nn} - \beta^{\mathrm{T}} K_1^{-1}\alpha)^{-1} K_1^{-1}\alpha\beta^{\mathrm{T}} K_1^{-1}$ has non-negative elements.

This completes the proof. □

From the above Theorem, together with the Perron-Frobenius Theorem for nonnegative matrices, we can deduce the following result.

Theorem 5. *Let G be a graph on n vertices with associated nonnegative symmetric matrix M, and let $K \in \mathcal{P}(n)$ with non-positive off-diagonal entries. If $K^{-1}M$ is irreducible, then the (M,K)-spectral radius $\rho(M,K)$ is simple and there exists an extensional eigenvector corresponding to $\rho(M,K)$ whose entries are all positive.*

Let G be a graph on n vertices and H an induced subgraph of G. For a matrix $K \in \mathcal{P}(n)$, the matrix $K(H)$ is the principal submatrix whose rows and columns correspond to the vertices of H. In what follows we present the result similar to the famous interlacing theorem.

Theorem 6. *Let G be a graph, H an induced subgraph of G and $K \in \mathcal{P}(n)$. If $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ are $(A(G),K)$-eigenvalues of G and $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_m$ are $(A(H),K(H))$-eigenvalues of H, then $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for any $1 \leq i \leq m$.*

Proof. Let $Q = (I_m \mid 0_{m\times n-m})^{\mathrm{T}}$. It is clear that $A(H) = Q^{\mathrm{T}} A(G) Q$ and $K(H) = Q^{\mathrm{T}} K Q$. Assume that $x_1, x_2, \ldots, x_m$ are $K(H)$-orthonormal extensional eigenvectors, that is $A(H)x_i = \mu_i K(H)x_i$ for $1 \leq i \leq m$ and $x_i^{\mathrm{T}} K(H) x_j = 1$ if $i = j$ and 0 otherwise. It yields that

$$\mu_i = \frac{x_i^{\mathrm{T}} A(H) x_i}{x_i^{\mathrm{T}} K(H) x_i} = \frac{(Qx_i)^{\mathrm{T}} A(G)(Qx_i)}{(Qx_i)^{\mathrm{T}} K(Qx_i)}.$$

Let $U = \langle Qx_i, Qx_{i+1}, \ldots, Qx_m \rangle$. For any $x \in U$, there exist $a_i, \ldots, a_m \in \mathbb{R}$ such that $x = \sum_{k=i}^m a_k Q x_k$. It leads to that

$$\begin{aligned} \frac{x^{\mathrm{T}} A(G) x}{x^{\mathrm{T}} K x} &= \frac{(\sum_{k=i}^m a_k Q x_k)^{\mathrm{T}} A(G)(\sum_{k=i}^m a_k Q x_k)}{(\sum_{k=i}^m a_k Q x_k)^{\mathrm{T}} K(\sum_{k=i}^m a_k Q x_k)} \\ &= \frac{(\sum_{k=i}^m a_k x_k)^{\mathrm{T}} (Q^{\mathrm{T}} A(G) Q)(\sum_{k=i}^m a_k x_k)}{(\sum_{k=i}^m a_k x_k)^{\mathrm{T}} (Q^{\mathrm{T}} K Q)(\sum_{k=i}^m a_k x_k)} \\ &= \frac{(\sum_{k=i}^m a_k x_k)^{\mathrm{T}} A(H)(\sum_{k=i}^m a_k x_k)}{(\sum_{k=i}^m a_k x_k)^{\mathrm{T}} K(H)(\sum_{k=i}^m a_k x_k)} \\ &= \frac{\sum_{k=i}^m a_k^2 \mu_k}{\sum_{k=i}^m a_k^2} \leq \mu_i. \end{aligned}$$

According to Theorem 2, we have

$$\lambda_{n-m+i} \leq \max_{x \in U} \frac{x^{\mathrm{T}} A(G) x}{x^{\mathrm{T}} K x} \leq \mu_i.$$

One can verify that $\lambda_i \geq \mu_i$ similarly by considering $-A(G)$. □

5. Further research

We should remark that most results in this paper can be generalized to the matrices in the complex field $\mathbb{C}$. We may take M to be Hermitian, and K to be Hermitian positive definite.

Since M is any symmetric matrix associate with a graph G, we could similarly discuss the distance type matrices such as the distance matrix, the distance Laplacian matrix, and so on. Also, the weighted graphs can be discussed similarly.

For a graph G and a non-bipartite graph G', by taking $M = A(G)$ and $K = Q(G')$, the (M, K)-sepctrum of G is called the *associated spectrum* of G with respect to G'. It is interesting to invesitgate that how the associated spectrum reveals the properties of these two graphs.

The characteristic polynomial of the adjacency matrix $A(G)$ of G is $f(x) = \det(xI - A(G)) = (x - \lambda_1)(x - \lambda_2)\dots(x - \lambda_n)$ where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are A-eigenvalues of G. For a graph G with adjacency matrix A and a matrix $K \in \mathcal{P}(n)$, the extensional characteristic polynomial of G with respect to K is defined as $f(x) = \det(xK - A)$. If $\lambda^{(K)}$ is an extensional eigenvalue then there exists $0 \neq x$ such that $Ax = \lambda^{(K)}Kx$, and thus $(\lambda^{(K)}K - A)x = 0$. It means that $\det(\lambda^{(K)}K - A) = 0$. Thus, $f(x) = \det K \cdot (x - \lambda_1^{(K)})(x - \lambda_2^{(K)})\dots(x - \lambda_n^{(K)})$ where $\lambda_1^{(K)} \geq \lambda_2^{(K)} \geq \dots \geq \lambda_n^{(K)}$ are (A, K)-eigenvalues. Since the values of the (A, K)-eigenvalues are dependent on K, the coefficients of $f(x)$ depend on K. We propose the following problems.

(i) Can the coefficients be expressed by the structure of G and the matrix K?
(ii) Characterize the bipartite graphs by using $(A(G), K)$-eigenvalues.
(iii) For general $K \in \mathcal{P}(n)$, determine the graph maximizing or minimizing the spectral radius $\rho(A, K)$ and characterize the corresponding extremal graphs.
(iv) If we take $M = A(G)$, can we find more properties of the $(A(G), K(G))$-eigenvalues?
(v) In this paper, we only consider the case for K being positive definite. What happens when K is only non-sigular, or even sigular ?

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