Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

BOUNDS ON THE SPECTRAL RADIUS OF GRAPHS VIA SUBGRAPH DELETION AND COALESCENCE*

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Abstract. The spectral radius of a graph is a fundamental parameter closely linked to network dynamics and robustness. Understanding its precise variation under structural perturbations such as vertex deletion, edge removal, or graph coalescence is a central problem in spectral graph theory. In this paper, we establish several sharp upper bounds that quantify these changes with an explicit dependence on local graph structures. For the deletion of an arbitrary nonempty proper vertex set S, we give an exact Schur-complement formula for $\rho(G)$ in terms of $G[S]$, $G-S$, and the incidence matrix between them. The formula gives a precise relation between the spectral radius before and after deleting S and yields a sharp upper bound with an equality characterization. In the special case where S is a clique, this gives an explicit clique-deletion estimate. We also derive an alternative local bound for graph coalescence that captures the degrees at the identified root and is sometimes sharper than the bound of Wang and Guo [(2020) *Linear Algebra Appl.*, 601:101–112, 2020.]. For the deletion of the endpoints of an edge, we obtain a bound that incorporates the number of triangles containing the specified edge. We characterize equality in these upper bounds.

Key words. Structural perturbation, Spectral radius, Bound.

AMS subject classifications. 05C50.

1. Introduction.

All graphs considered in this paper are finite, undirected, and simple. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Its *order* is n, and its *size* is m. Let $A(G)$ be the adjacency matrix of G. Since $A(G)$ is a real symmetric matrix, all of its eigenvalues are real. We order them as $\lambda_1(A(G)) \geq \lambda_2(A(G)) \geq \cdots \geq \lambda_n(A(G))$. The largest eigenvalue $\lambda_1(A(G))$, denoted by $\rho(G)$, is called the *spectral radius* of G. Note that $A(G)$ is nonnegative and is irreducible if and only if G is connected. Therefore, when G is a connected graph with at least two vertices, the Perron–Frobenius theorem implies that $\rho(G)$ is strictly positive, its multiplicity is one, and there exists a unique strictly positive unit eigenvector $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^T$, known as the Perron vector of G.

The spectral radius of a graph is closely related to its topological and dynamical properties (see, *e.g.*, [1, 2]). A fundamental problem in spectral graph theory is to quantify the change in the spectral radius under structural perturbations such as vertex deletion and edge deletion. Removing an edge or a vertex from a graph cannot increase its spectral radius. For a connected graph with at least two vertices, the Perron–Frobenius theorem shows that either operation strictly decreases the spectral radius. A natural question is how to estimate this decrease in terms of the local structure at the removed edge or vertex. Van Mieghem *et al.* [9] and Li *et al.* [5] obtained quantitative bounds on the decrease of the spectral radius after such removals.

*Received by the editors on June 24, 2026. Accepted for publication on September 16, 2026. Handling Editor: Michael Tait. Corresponding Author: Jianxi Li.

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Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

We study how local adjacency information controls the spectral radius under subgraph deletion and graph coalescence. Our results concern the following three settings.

- We study deletion of an arbitrary nonempty proper vertex set by means of a Schur-complement formula. This gives an exact equation for $\rho(G)$ in terms of $G[S]$, $G-S$ and the edges between them, as well as an explicit upper bound with equality characterized. When the deleted set is a clique, the formula gives an explicit clique-deletion estimate.
- We derive an alternative local bound for the coalescence of two rooted graphs, using the degrees at the identified root. This bound is sometimes sharper than the global bound of Wang and Guo [10], as illustrated in Example 2.9.
- For the deletion of the endpoints of an edge, we give a bound that explicitly involves the number of triangles containing that edge. This estimate uses different data from the universal bound for deleting the edge itself; we state an explicit comparison condition in Remark 2.12.

We also characterize equality in the resulting upper bounds.

2. Preliminaries and main results. Before stating the main results, we introduce some terminology and notation. For any vertex $v \in V(G)$, let $d_G(v)$ and $N_G(v)$ (or $d(v)$ and $N(v)$ for short) be the degree and the set of neighbors of v, respectively. Clearly, $d_G(v) = |N_G(v)|$. For $e \in E(G)$ (or $v \in V(G)$), let $G-e$ (or $G-v$) be the graph obtained from G by deleting the edge e (or the vertex v). For a subset $S \subseteq V(G)$, let $G[S]$ denote the subgraph of G induced by S, and let $G-S$ denote the subgraph obtained by deleting the vertices in S together with their incident edges. For $S, T \subseteq V(G)$ with $S \cap T = \emptyset$, let $E(S,T) = \{uv \in E(G) : u \in S, v \in T\}$ and $e(S,T) = |E(S,T)|$. Let A and B be two symmetric matrices. We write $B \preceq A$ if $A - B$ is positive semidefinite. We use the convention $\rho(\emptyset) = 0$ when all vertices are deleted.

2.1. Vertex deletion. Recently, the relationship between $\rho(G)$ and $\rho(G-v)$ has been widely studied. Guo, Wang, and Li [3] established an upper bound for $\rho(G)$ in terms of $\rho(G-v)$ and the degree $d(v)$, and proposed a stronger conjecture. Sun and Das [8] subsequently confirmed this conjecture by proving Theorem 2.1 below. Liu and Ning [6] later provided a short, self-contained proof.

THEOREM 2.1 ([8]). *Let G be a connected graph of order n. For any $v \in V(G)$ with $d(v) \geq 1$, we have*

$$\rho(G) \leq \sqrt{\rho^2(G-v) + 2d(v) - 1}.$$

Equality holds if and only if either $G \cong K_{1,n-1}$ and v is a pendant vertex, or $G \cong K_n$.

We next record an exact formula for deleting a vertex set. Let S be a nonempty proper subset of $V(G)$, and order the vertices with those in S first and those in $V(G) \setminus S$ second. With respect to this ordering, the adjacency matrix has the block form

$$A(G) = \begin{pmatrix} A(G[S]) & C \\ C^T & A(G-S) \end{pmatrix},$$

where C is the $|S| \times |V(G) \setminus S|$ incidence matrix between the two vertex sets: its (x,y)-entry is 1 if $xy \in E(G)$ and 0 otherwise.

THEOREM 2.2. *Let G be a connected graph, and let $\emptyset \neq S \subsetneq V(G)$. Then, $\rho(G)$ is the unique solution in $(\rho(G-S), \infty)$ of*

$$\lambda = \lambda_1\left(A(G[S]) + C(\lambda I - A(G-S))^{-1}C^T\right).$$

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Moreover,

$$\rho(G) \leq \frac{\rho(G-S)+\rho(G[S])+\sqrt{(\rho(G-S)-\rho(G[S]))^2+4e(S,V(G)\setminus S)}}{2}.$$

Equality in this bound holds if and only if every vertex of S is adjacent to every vertex of $V(G)\setminus S$, and both $G[S]$ and $G-S$ are regular.

Taking S to be a clique gives the following exact deletion formula.

COROLLARY 2.3. *Let G be a connected graph, and let $S \subsetneq V(G)$ with $G[S] \cong K_k$, where $k \geq 1$. Let C be the incidence matrix between S and $V(G)\setminus S$. Then, $\rho(G)$ is the unique solution in $(\rho(G-S),\infty)$ of*

$$\lambda = \lambda_1\left(J_k - I_k + C(\lambda I - A(G-S))^{-1}C^T\right),$$

where J_k is the all-one matrix of order k. Moreover,

$$\rho(G) \leq \frac{\rho(G-S)+k-1+\sqrt{(\rho(G-S)-k+1)^2+4e(S,V(G)\setminus S)}}{2}.$$

Equality in this bound holds if and only if every vertex of S is adjacent to every vertex of $V(G)\setminus S$, and $G-S$ is regular. When $S=V(K_k)$, the same bound can be written with $G-S=G-K_k$ and $e(S,V(G)\setminus S) = e(V(K_k),V(G-K_k))$.

In particular, for $k=1$, we have the following corollary.

COROLLARY 2.4. *Let G be a connected graph of order $n \geq 2$. For $v \in V(G)$, we have*

$$\rho(G) \leq \frac{\rho(G-v)+\sqrt{\rho^2(G-v)+4d(v)}}{2}.$$

Moreover, equality holds if and only if $G \cong K_1 \vee H$ and v is the vertex in the K_1 factor, where H is a regular graph of order $n-1$.

Remark 2.5. It can be checked that

$$\frac{\rho(G-v)+\sqrt{\rho^2(G-v)+4d(v)}}{2} \leq \sqrt{\rho^2(G-v)+2d(v)-1}$$

for $d(v) \geq 1+\rho(G-v)$. Hence, the bound in Corollary 2.4 is at least as good as that in Theorem 2.1 when $d(v) \geq 1+\rho(G-v)$.

2.2. Coalescence. Theorem 2.1 and Corollary 2.3 bound the spectral radius using the remaining subgraph and the edges incident with the deleted vertices. A related question is whether the local degrees at a root can also give useful bounds when two rooted graphs are joined at that root.

The notation (G,u) means that G is a rooted graph and $u \in V(G)$ is labeled as a root. Let (H,u) and (K,w) be two rooted graphs. The coalescence $G=(H,u)*(K,w)$ is formed from disjoint copies of H and K by identifying the roots u and w. Recently, Wang and Guo [10] investigated upper bounds for the spectral radius of coalesced graphs, generalizing the results of Passbani and Salemi [7].

THEOREM 2.6 ([10]). *Let (H,v) and (K,w) be two non-trivial connected rooted graphs. Then,*

$$\rho((H,v)*(K,w)) \leq \sqrt{\rho^2(H)+\rho^2(K)},$$

with equality if and only if $(H,v)*(K,w)$ is a star.

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Theorem 2.6 provides a global bound $\sqrt{\rho^2(H)+\rho^2(K)}$ that does not reflect the local degrees at the identified root. The following theorem gives an alternative local bound in terms of these degrees and the spectral radii of the graphs obtained by deleting the roots. It is sometimes sharper than Theorem 2.6, but neither bound dominates the other in general.

THEOREM 2.7. *Let $G=(H,u)*(K,w)$, where (H,u) and (K,w) are two non-trivial connected rooted graphs. Then, we have*

$$1 \le \frac{2d_H(u)-1}{\rho^2(G)-\rho^2(H-u)} + \frac{2d_K(w)-1}{\rho^2(G)-\rho^2(K-w)}. \tag{2.1}$$

Moreover, let $\mu_{\max}=\max\{\rho(H-u),\rho(K-w)\}$. Then we have

$$\rho(G) \le \sqrt{\mu_{\max}^2+2(d_H(u)+d_K(w))-2}. \tag{2.2}$$

Equality in (2.2) holds if and only if $\rho(H-u)=\rho(K-w)$, and both H and K are stars with u,w as leaves, respectively.

Remark 2.8. The identified vertex v is a cut vertex of G, with $d_G(v)=d_H(u)+d_K(w)$. Applying Theorem 2.1 directly to v gives

$$\rho(G) \le \sqrt{\mu_{\max}^2+2(d_H(u)+d_K(w))-1},$$

where $\mu_{\max}=\max\{\rho(H-u),\rho(K-w)\}$. Thus, (2.2) strictly improves this direct application by reducing the constant term from -1 to -2. This comparison is with Theorem 2.1 applied to G, not with Theorem 2.6.

Example 2.9. Let H and K be two copies of the star $K_{1,k}$ ($k\ge 2$). Choose a leaf u in H and a leaf w in K, and let $G=(H,u)*(K,w)$ be the graph obtained by identifying u and w into a single cut vertex v. The spectral radius of a star $K_{1,k}$ is $\sqrt{k}$, so $\rho(H)=\rho(K)=\sqrt{k}$. Theorem 2.6 gives the bound

$$\rho(G) \le \sqrt{\rho^2(H)+\rho^2(K)} = \sqrt{2k}.$$

We now apply Theorem 2.7. Removing the leaf u from H leaves the star $K_{1,k-1}$, so $\rho(H-u)=\sqrt{k-1}$. The same holds for $K-w$, so $\mu_{\max}=\sqrt{k-1}$. Since $d_H(u)=d_K(w)=1$, the bound in Theorem 2.7 becomes

$$\rho(G) \le \sqrt{\mu_{\max}^2+2(1+1)-2} = \sqrt{(k-1)+2} = \sqrt{k+1}.$$

To see the exact value of $\rho(G)$, write the eigenvector equations for the Perron vector of G. By symmetry, all leaves have the same entry x_l, both centers have the same entry x_c, and the cut vertex has entry x_v. The eigenvalue equations are

$$\begin{cases} \rho(G)x_l = x_c, \\ \rho(G)x_c = (k-1)x_l + x_v, \\ \rho(G)x_v = 2x_c. \end{cases}$$

Substituting $x_l=\frac{x_c}{\rho(G)}$ and $x_v=\frac{2x_c}{\rho(G)}$ into the second equation yields

$$\rho(G)x_c = (k-1)\frac{x_c}{\rho(G)} + \frac{2x_c}{\rho(G)} = \frac{k+1}{\rho(G)}x_c.$$

It follows that $\rho(G)^2=k+1$. Hence, $\rho(G)=\sqrt{k+1}$. For this family of graphs, Theorem 2.7 attains equality, while Theorem 2.6 gives the strictly larger bound $\sqrt{2k}$. For example, taking $k=10$ gives $\rho(G)=\sqrt{11}\approx 3.317$; Theorem 2.6 gives $\sqrt{20}\approx 4.472$.

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A publication of the International Linear Algebra Society
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The reverse comparison occurs when the centers, rather than leaves, of two copies of $K_{1,k}$ are identified. The resulting graph is $K_{1,2k}$, for which Theorem 2.6 gives the exact value $\sqrt{2k}$, whereas (2.2) gives the strictly larger bound $\sqrt{4k-2}$ for $k \geq 2$.

2.3. Deletion of the endpoints of an edge. Van Mieghem *et al.* [9] showed that $\rho(G) \leq \rho(G-e)+1$ for every $e \in E(G)$. The next bound uses the spectral radius after deleting both endpoints of e, rather than after deleting e alone. It also incorporates the number of triangles $t(e)$ containing the specified edge. Since these bounds use different remaining subgraphs, we do not claim that the new bound is uniformly sharper.

THEOREM 2.10. *Let G be a connected graph, and let $e = uv$ be an edge of G. Let $t(e)$ be the number of triangles containing the edge e, and let $G_{uv} = G - \{u, v\}$ be the induced subgraph obtained by deleting vertices u and v. Write $d_u = d_G(u)$ and $d_v = d_G(v)$ and define the local structure matrix*

$$D_e = \begin{pmatrix} d_u - 1 & t(e) \\ t(e) & d_v - 1 \end{pmatrix}.$$

Let λ_D be the largest eigenvalue of D_e. Then,

$$\rho(G) \leq \frac{\rho(G_{uv}) + 1 + \sqrt{(\rho(G_{uv}) - 1)^2 + 4\lambda_D}}{2},$$

with equality if and only if all the following conditions are satisfied:

(i) $d_G(u) = d_G(v)$;
(ii) For every vertex $x \in V(G_{uv})$, we have

$$\sum_{y \in N_{G_{uv}}(x)} c(y) = \rho(G_{uv}) c(x),$$

where $c(x)$ is the number of edges connecting the vertex $x \in V(G_{uv})$ to the set $\{u, v\}$.

Example 2.11. Let $G = K_n$ $(n \geq 4)$ and $e = uv \in E(K_n)$. Then, $\rho(G) = n-1$, $d_G(u) = d_G(v) = n-1$, $t(e) = n-2$, and $G_{uv} = K_{n-2}$ with $\rho(G_{uv}) = n-3$. The matrix D_e has entries $n-2$ and maximum eigenvalue $\lambda_D = 2n-4$.

The bound $\rho(G) \leq \rho(G-e)+1$ gives $\rho(K_4) \leq (3+\sqrt{17})/2 \approx 3.562$ when $n = 4$, whereas Theorem 2.10 yields

$$\rho(G) \leq \frac{(n-3)+1+\sqrt{((n-3)-1)^2 + 4(2n-4)}}{2} = \frac{n-2+n}{2} = n-1.$$

Thus, Theorem 2.10 attains equality on these complete graphs, while the constant bound is strictly weaker. Indeed, $K_n - e$ is connected and contains K_{n-1} as a proper subgraph, so $\rho(K_n - e) > n-2$.

Remark 2.12. Deleting the edge uv leaves both endpoints in the graph, unlike the removal of $\{u, v\}$ as a clique of size 2. For $|V(G)| \geq 3$, applying Corollary 2.3 with $k = 2$ to delete u and v gives

$$\rho(G) \leq \frac{\rho(G_{uv}) + 1 + \sqrt{(\rho(G_{uv}) - 1)^2 + 4(d_G(u) + d_G(v) - 2)}}{2}.$$

For the complete graph $G = K_n$ with $n \geq 3$, this bound is

$$\frac{n-2+\sqrt{(n-4)^2 + 8(n-2)}}{2} = n-1,$$

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A publication of the International Linear Algebra Society
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so it is tight. Since $D_e = B^T B$ is positive semidefinite, where B is the incidence matrix used in Section 5, $\lambda_D \leq \mathrm{tr}(D_e) = d_G(u) + d_G(v) - 2$. Thus, Theorem 2.10 refines this clique-deletion bound by retaining the largest eigenvalue of D_e rather than its trace. This comparison does not imply a uniform improvement over the edge-deletion bound $\rho(G-e)+1$.

For an explicit comparison with that bound, put $\mu = \rho(G_{uv})$ and $\beta = \rho(G-e)$. Since $\beta \geq \mu$, the upper bound in Theorem 2.10 is at most $\beta+1$ if and only if

$$\lambda_D \leq \beta(\beta + 1 - \mu).$$

Indeed, the bound in Theorem 2.10 is the larger root of $(z-1)(z-\mu) = \lambda_D$, and $(z-1)(z-\mu)$ is strictly increasing for $z > \max\{1, \mu\}$. Also, $\beta+1 \geq \max\{1, \mu\}$. The comparison is strict precisely when the displayed inequality is strict.

3. Proofs of Theorem 2.2 and Corollary 2.3. We prove Theorem 2.2 first and then deduce Corollary 2.3.

Proof of Theorem 2.2: Let $\rho = \rho(G)$, and let $\boldsymbol{x} = (\boldsymbol{x}_S^T, \boldsymbol{x}_{V(G)\setminus S}^T)^T$ be the Perron vector of G, written according to this ordering. Since G is connected and $G - S$ is a proper subgraph, $\rho > \rho(G-S)$. Hence, $\rho I - A(G-S)$ is nonsingular. The eigenvalue equation $A(G)\boldsymbol{x} = \rho\boldsymbol{x}$ gives

$$A(G[S])\boldsymbol{x}_S + C\boldsymbol{x}_{V(G)\setminus S} = \rho\boldsymbol{x}_S, \tag{3.1}$$

$$C^T\boldsymbol{x}_S + A(G-S)\boldsymbol{x}_{V(G)\setminus S} = \rho\boldsymbol{x}_{V(G)\setminus S}. \tag{3.2}$$

By (3.2), we have

$$\boldsymbol{x}_{V(G)\setminus S} = (\rho I - A(G-S))^{-1}C^T\boldsymbol{x}_S.$$

Substitution of this expression into (3.1) yields

$$\left(A(G[S]) + C(\rho I - A(G-S))^{-1}C^T\right)\boldsymbol{x}_S = \rho\boldsymbol{x}_S.$$

For $\lambda > \rho(G-S)$, the Neumann series

$$(\lambda I - A(G-S))^{-1} = \frac{1}{\lambda}\sum_{j=0}^{\infty}\left(\frac{A(G-S)}{\lambda}\right)^j,$$

converges and has nonnegative entries. Hence, the matrix $A(G[S]) + C(\rho I - A(G-S))^{-1}C^T$ is nonnegative and has the positive eigenvector $\boldsymbol{x}_S$. Conjugating this matrix by the diagonal matrix with diagonal $\boldsymbol{x}_S$ gives a nonnegative matrix whose row sums all equal ρ. Its spectral radius is therefore ρ, whether or not it is irreducible. Since the original matrix is symmetric, we conclude that

$$\rho = \lambda_1\left(A(G[S]) + C(\rho I - A(G-S))^{-1}C^T\right).$$

Thus, ρ satisfies the displayed equation in the theorem.

It remains to prove uniqueness. The symmetric matrix $A(G-S)$ has an orthonormal eigenbasis. On an eigenspace with eigenvalue θ, the resolvent $(\lambda I - A(G-S))^{-1}$ acts as multiplication by $(\lambda-\theta)^{-1}$. This

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
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scalar is positive and strictly decreasing for $\lambda > \rho(G-S)$, since $\theta \le \rho(G-S)$. Thus, if $\rho(G-S) < \alpha < \beta$, then

$$(\beta I - A(G-S))^{-1} \preceq (\alpha I - A(G-S))^{-1}.$$

Congruence by C preserves this order, as does taking the largest eigenvalue after adding $A(G[S])$. Thus, the right-hand side of the equation is nonincreasing on $(\rho(G-S), \infty)$. The difference between the left-hand side and the right-hand side is therefore strictly increasing there, so the equation has at most one solution.

We next prove the displayed bound. Write $\lambda = \rho(G)$, $\mu = \rho(G-S)$, and $\alpha = \rho(G[S])$. Since $\lambda > \mu$,

$$(\lambda I - A(G-S))^{-1} \preceq \frac{1}{\lambda - \mu} I.$$

Also $\lambda > \alpha$, since $G[S]$ is a proper subgraph of the connected graph G. Using the exact formula just proved, we obtain

$$\lambda \le \alpha + \frac{\lambda_1(CC^T)}{\lambda - \mu} \le \alpha + \frac{e(S, V(G) \setminus S)}{\lambda - \mu}.$$

Hence,

$$(\lambda - \alpha)(\lambda - \mu) \le e(S, V(G) \setminus S),$$

and solving this quadratic inequality gives the stated upper bound.

Suppose first that equality holds in the bound. Then, equality holds throughout the preceding inequalities. In particular, $\lambda_1(CC^T) = \mathrm{tr}(CC^T)$. Thus, C has rank one. Since C is a nonzero $0,1$ matrix, there are nonempty sets $X \subseteq S$ and $Y \subseteq V(G) \setminus S$ such that the ones of C occur exactly in $X \times Y$.

The Perron vector $\boldsymbol{x}_S$ is positive. Equality in $\lambda_1(A(G[S]) + M) \le \rho(G[S]) + \lambda_1(M)$ and $M = C(\lambda I - A(G-S))^{-1}C^T$ forces $\boldsymbol{x}_S$ to be an eigenvector belonging to the largest eigenvalue of each of $A(G[S])$ and M. Since C has the form described above, M is a positive multiple of the matrix whose principal block on X is all-one and whose other entries are zero. The positivity of $\boldsymbol{x}_S$ therefore gives $X = S$. It follows that all rows of C are equal. The same equality also gives $\boldsymbol{x}_S$ proportional to the all-one vector on S, and hence $A(G[S])\mathbf{1} = \alpha\mathbf{1}$. Thus, $G[S]$ is regular.

Equality in

$$(\lambda I - A(G-S))^{-1} \preceq \frac{1}{\lambda - \mu} I,$$

when evaluated at $C^T\boldsymbol{x}_S$, which is a nonzero multiple of $\mathbf{1}_Y$, gives

$$A(G-S)\mathbf{1}_Y = \mu\mathbf{1}_Y.$$

Thus, Y is a union of components of $G-S$, each regular of degree μ. Since the columns of C outside Y are zero, no vertex of $(V(G) \setminus S) \setminus Y$ is adjacent to S. The last displayed equality also shows that there are no edges between Y and $(V(G) \setminus S) \setminus Y$. As G is connected, we must have $Y = V(G) \setminus S$. Hence, every vertex of S is adjacent to every vertex of $V(G) \setminus S$, and $G-S$ is regular.

Conversely, suppose that every vertex of S is adjacent to every vertex of $V(G) \setminus S$, and that both $G[S]$ and $G-S$ are regular. Let $s = |S|$ and $h = |V(G) \setminus S|$. Then, $C = J_{s,h}$, the all-one $s \times h$ matrix. Moreover, if $\mu = \rho(G-S)$, then

$$(\lambda I - A(G-S))^{-1}\mathbf{1}_h = \frac{1}{\lambda - \mu}\mathbf{1}_h.$$

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Hence, $C(\lambda I - A(G-S))^{-1}C^T = \frac{h}{\lambda-\mu}J_s$. Since $G[S]$ is regular with degree $\rho(G[S])$, the exact equation reduces to

$$\lambda = \rho(G[S]) + \frac{sh}{\lambda-\mu}.$$

As $sh = e(S, V(G)\backslash S)$, this is exactly the quadratic equation corresponding to the displayed bound. Equality follows. This proves the theorem. □

Proof of Corollary 2.3: Since $G[S] \cong K_k$, we have $A(G[S]) = J_k - I_k$ and $\rho(G[S]) = k-1$. The exact equation, the displayed bound, and the equality condition therefore follow at once from Theorem 2.2. □

4. Proof of Theorem 2.7. We need the following lemmas to prove Theorem 2.7.

LEMMA 4.1 ([2]). *For any graph G of order $n \geq 1$ and size m, with maximum degree Δ, $\frac{2m}{n} \leq \rho(G) \leq \Delta$.*

LEMMA 4.2 ([1]). *Let G be a connected graph with at least two vertices. If H is a spanning subgraph of G, then $\rho(H) \leq \rho(G)$, with equality if and only if $G = H$. Moreover, if H is a proper subgraph of G, then $\rho(H) < \rho(G)$.*

LEMMA 4.3. *For a real symmetric $n \times n$ matrix B, let $\rho(B)$ be its spectral radius. Then, for $\lambda > \rho(B)$, the matrix $\lambda I - B$ is positive definite and*

$$(\lambda I - B)^{-1} \preceq \frac{\lambda I + B}{\lambda^2 - \rho(B)^2}.$$

Moreover, for any vector $\boldsymbol{b} \in \mathbb{R}^n$, we have

$$\boldsymbol{b}^T(\lambda I - B)^{-1}\boldsymbol{b} = \boldsymbol{b}^T\Big(\frac{\lambda I + B}{\lambda^2 - \rho(B)^2}\Big)\boldsymbol{b} \iff B^2\boldsymbol{b} = \rho(B)^2\boldsymbol{b}.$$

Proof. Since B is a real symmetric matrix, there exists an orthogonal matrix U satisfying $U^TU = I$ and a diagonal matrix $\Lambda = \mathrm{diag}(t_1, t_2, \ldots, t_n)$ such that $B = U\Lambda U^T$, where t_i are the eigenvalues of B. By definition, all eigenvalues satisfy $t_i \leq \rho(B) < \lambda$. Construct the matrix difference

$$M = \frac{\lambda I + B}{\lambda^2 - \rho(B)^2} - (\lambda I - B)^{-1}.$$

Substituting the orthogonal decomposition into M and extracting the common factors yields

$$M = U\left(\frac{\lambda I + \Lambda}{\lambda^2 - \rho(B)^2} - (\lambda I - \Lambda)^{-1}\right)U^T.$$

The matrix in the middle is a diagonal matrix. Its i-th diagonal entry is

$$\frac{\lambda + t_i}{\lambda^2 - \rho(B)^2} - \frac{1}{\lambda - t_i} = \frac{(\lambda + t_i)(\lambda - t_i) - (\lambda^2 - \rho(B)^2)}{(\lambda^2 - \rho(B)^2)(\lambda - t_i)} = \frac{\rho(B)^2 - t_i^2}{(\lambda^2 - \rho(B)^2)(\lambda - t_i)}.$$

Since t_i is an eigenvalue with $|t_i| \leq \rho(B)$, we have $\rho(B)^2 - t_i^2 \geq 0$. Meanwhile, since $\lambda > \rho(B) \geq |t_i|$, we have $(\lambda^2 - \rho(B)^2)(\lambda - t_i) > 0$. Hence, $M \succeq 0$.

For a given vector $\boldsymbol{b}$, the equality of the quadratic form is equivalent to $\boldsymbol{b}^TM\boldsymbol{b} = 0$. Since M is positive semidefinite, this condition is equivalent to $M\boldsymbol{b} = 0$. The diagonalization above shows that every nonzero projection of $\boldsymbol{b}$ onto an eigenspace of B must correspond to an eigenvalue t_i with $\rho(B)^2 - t_i^2 = 0$, that is, $t_i^2 = \rho(B)^2$. This is equivalent to $(B^2 - \rho(B)^2 I)\boldsymbol{b} = 0$, or $B^2\boldsymbol{b} = \rho(B)^2\boldsymbol{b}$. □

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A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

We now prove Theorem 2.7, using an argument similar to that in [6].

Proof of Theorem 2.7: Let v be the vertex obtained by identifying u and w. Order the adjacency matrix $A(G)$ with v first. Then, $G-v$ is the disjoint union of $H-u$ and $K-w$; either of these graphs may itself be disconnected. Let $\boldsymbol{b}_H$, $\boldsymbol{b}_K$ be the column vectors representing connections from v to $H-u$ and $K-w$, respectively. Thus, $\boldsymbol{b}_H^T\boldsymbol{b}_H = d_H(u)$ and $\boldsymbol{b}_K^T\boldsymbol{b}_K = d_K(w)$. The matrix $A(G)$ has the form

$$A(G) = \begin{pmatrix} 0 & \boldsymbol{b}_H^T & \boldsymbol{b}_K^T \\ \boldsymbol{b}_H & A(H-u) & 0 \\ \boldsymbol{b}_K & 0 & A(K-w) \end{pmatrix}.$$

Let $\rho = \rho(G)$. Since G is connected and both rooted graphs are non-trivial, Lemma 4.2 gives $\rho > \max\{\rho(H-u), \rho(K-w)\}$. The relevant resolvents therefore exist. The equation $\det(\rho I - A(G)) = 0$ gives, by the Schur complement,

$$\rho = \boldsymbol{b}_H^T(\rho I - A(H-u))^{-1}\boldsymbol{b}_H + \boldsymbol{b}_K^T(\rho I - A(K-w))^{-1}\boldsymbol{b}_K. \tag{4.1}$$

Apply Lemma 4.3 to each term with $\lambda = \rho$. For $\boldsymbol{b}_H$, this gives

$$\boldsymbol{b}_H^T(\rho I - A(H-u))^{-1}\boldsymbol{b}_H \leq \frac{\rho\boldsymbol{b}_H^T\boldsymbol{b}_H + \boldsymbol{b}_H^T A(H-u)\boldsymbol{b}_H}{\rho^2 - \rho^2(H-u)}. \tag{4.2}$$

Define $m_H = \boldsymbol{b}_H^T A(H-u)\boldsymbol{b}_H = 2e(H[N_H(u)])$. Consider the induced subgraph $F_H = H[\{u\} \cup N_H(u)]$. It has $d_H(u)+1$ vertices and $d_H(u) + m_H/2$ edges. Its average degree is

$$\bar{d}(F_H) = \frac{2d_H(u) + m_H}{d_H(u)+1}.$$

Notice that for any $d_H(u) \geq 1$, by Lemmas 4.1 and 4.2, we have $\rho \geq \rho(F_H) \geq \bar{d}(F_H)$. If $d_H(u) \geq 2$, then F_H is a proper induced subgraph of the connected graph G, because K is non-trivial. By Lemma 4.2, $\rho(F_H) < \rho(G)$. Thus, we have

$$\rho > \rho(F_H) \geq \bar{d}(F_H) = \frac{2d_H(u) + m_H}{d_H(u)+1}. \tag{4.3}$$

We claim that $m_H \leq \rho(d_H(u)-1)$ in all cases, with strict inequality when $d_H(u) \geq 2$. If $d_H(u) = 1$, then $m_H = 0$ and $d_H(u) - 1 = 0$, so $m_H \leq \rho\,(d_H(u)-1)$ trivially holds. If $d_H(u) \geq 2$, we compute

$$\frac{2d_H(u) + m_H}{d_H(u)+1} - \frac{m_H}{d_H(u)-1} = \frac{2[d_H(u)(d_H(u)-1) - m_H]}{d_H^2(u)-1} \geq 0,$$

where the non-negativity follows from $m_H \leq d_H(u)(d_H(u)-1)$. Combining this with the strict inequality (4.3) yields

$$\rho > \frac{m_H}{d_H(u)-1} \quad \Longrightarrow \quad m_H < \rho\,(d_H(u)-1), \tag{4.4}$$

as desired.

Substituting $\boldsymbol{b}_H^T\boldsymbol{b}_H = d_H(u)$ and $m_H \leq \rho(d_H(u)-1)$ into (4.2) yields

$$\boldsymbol{b}_H^T(\rho I - A(H-u))^{-1}\boldsymbol{b}_H \leq \frac{\rho d_H(u) + m_H}{\rho^2 - \rho^2(H-u)} \leq \frac{\rho(2d_H(u)-1)}{\rho^2 - \rho^2(H-u)}. \tag{4.5}$$

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A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

If $d_H(u) \geq 2$, the second inequality in (4.5) is strict. Similarly, for K,

$$\boldsymbol{b}_K^T(\rho I - A(K-w))^{-1}\boldsymbol{b}_K \leq \frac{\rho d_K(w) + m_K}{\rho^2 - \rho^2(K-w)} \leq \frac{\rho(2d_K(w)-1)}{\rho^2 - \rho^2(K-w)}, \tag{4.6}$$

where $m_K = \boldsymbol{b}_K^T A(K-w)\boldsymbol{b}_K$ and the second inequality is strict if $d_K(w) \geq 2$.

Substituting (4.5) and (4.6) into (4.1) and dividing by $\rho > 0$ gives

$$1 \leq \frac{2d_H(u)-1}{\rho^2 - \rho^2(H-u)} + \frac{2d_K(w)-1}{\rho^2 - \rho^2(K-w)},$$

which is (2.1).

Let $\mu_{\max} = \max\{\rho(H-u), \rho(K-w)\}$. Then, $\rho^2 - \rho^2(H-u) \geq \rho^2 - \mu_{\max}^2$ and similarly for $K-w$. Since the denominators in (2.1) are positive, replacing them by the smaller quantity $\rho^2 - \mu_{\max}^2$ increases the right-hand side. Hence,

$$1 \leq \frac{2d_H(u)-1+2d_K(w)-1}{\rho^2 - \mu_{\max}^2} = \frac{2(d_H(u)+d_K(w))-2}{\rho^2 - \mu_{\max}^2}.$$

Rearranging yields $\rho^2 \leq \mu_{\max}^2 + 2(d_H(u)+d_K(w)) - 2$, *i.e.*, (2.2).

Equality case. Assume equality holds in (2.2). Then, all inequalities in the chain are equalities. In particular,

- $\rho(H-u) = \rho(K-w) = \mu_{\max}$ (from the denominator replacement).
- $m_H = \rho\,(d_H(u)-1)$ and $m_K = \rho\,(d_K(w)-1)$.
- Equality in Lemma 4.3 gives $A(H-u)^2\boldsymbol{b}_H = \rho^2(H-u)\boldsymbol{b}_H$ and similarly for K.

As shown above, if $d_H(u) \geq 2$ or $d_K(w) \geq 2$, the second inequality in (4.5) or (4.6), respectively, would be strict. This would preclude equality in (2.2). Therefore, equality forces $d_H(u) = d_K(w) = 1$.

Now $d_H(u) = 1$ implies $\boldsymbol{b}_H$ has a single 1 at the coordinate of the unique neighbor u' of u in H. The equality condition $A(H-u)^2\boldsymbol{e}_{u'} = \rho^2(H-u)\boldsymbol{e}_{u'}$ means that for any vertex $x \neq u'$, $(A(H-u)^2)_{u',x} = 0$. Notice that $(A(H-u)^2)_{u',x} = \sum_z A_{u',z}A_{z,x} = 0$. Since the adjacency matrix is nonnegative, this implies that for any neighbor z of u' (i.e., $A_{u',z} = 1$), we must have $A_{z,x} = 0$ for all $x \neq u'$. In other words, no neighbor of u' can have any other neighbors besides u'. Because H is connected and u is a leaf, $H-u$ is connected. It must therefore be a star centered at u' (possibly consisting of the single vertex u'). Adding the leaf u gives that H is a star with leaf u. The same holds for K. Conversely, suppose that H and K are stars with u and w as leaves and that $\rho(H-u) = \rho(K-w) = \mu_{\max}$. In this case, $d_H(u) = d_K(w) = 1$, $m_H = m_K = 0$, and $A(H-u)^2\boldsymbol{b}_H = \mu_{\max}^2\boldsymbol{b}_H$, with the analogous identity for K. Equality in Lemma 4.3 and (4.1) then gives

$$\rho = \frac{\rho}{\rho^2 - \mu_{\max}^2} + \frac{\rho}{\rho^2 - \mu_{\max}^2}.$$

Since $\rho > 0$, we have $\rho^2 = \mu_{\max}^2 + 2$, which is equality in (2.2).

This completes the proof of Theorem 2.7. □

Electronic Journal of Linear Algebra, ISSN 1081-3810
A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

5. Proof of Theorem 2.10. In order to prove Theorem 2.10, we need the following lemma.

LEMMA 5.1 ([4]). *Let A and B be Hermitian matrices of the same order. Then,*

$$\lambda_1(A+B) \le \lambda_1(A) + \lambda_1(B).$$

Equality holds if and only if A and B have a common nonzero eigenvector belonging to $\lambda_1(A)$ and $\lambda_1(B)$, respectively.

Proof. Let $\boldsymbol{x}$ be a unit eigenvector of $A+B$ belonging to $\lambda_1(A+B)$. By the Rayleigh principle,

$$\lambda_1(A+B) = \boldsymbol{x}^* A\boldsymbol{x} + \boldsymbol{x}^* B\boldsymbol{x} \le \lambda_1(A) + \lambda_1(B),$$

where $\boldsymbol{x}^*$ denotes the conjugate transpose. Equality holds precisely when $\boldsymbol{x}$ attains the largest Rayleigh quotient of both matrices, that is, when $A\boldsymbol{x} = \lambda_1(A)\boldsymbol{x}$ and $B\boldsymbol{x} = \lambda_1(B)\boldsymbol{x}$. Conversely, a common eigenvector for these two largest eigenvalues gives the reverse inequality for $\lambda_1(A+B)$, and hence equality. ∎

Proof of Theorem 2.10: Let $G = (V, E)$ be a connected graph, and let $e = uv \in E$. If $G = K_2$, then $G_{uv} = \emptyset$, $D_e = 0$, and both sides of the bound equal 1; conditions (i) and (ii) also hold. We may therefore assume that $|V| \ge 3$. Set $\rho = \rho(G)$, and let $M = A(G_{uv})$ be the adjacency matrix of $G_{uv} = G - \{u, v\}$. We denote its maximum eigenvalue by $\mu = \rho(G_{uv})$. Since $G_{uv} \subsetneq G$ and G is connected, by Lemma 4.2, $\rho > \mu$. Partitioning the vertex set as $V = \{u, v\} \cup V(G_{uv})$, the adjacency matrix $A(G)$ admits the block representation

$$A(G) = \begin{pmatrix} U & B^T \\ B & M \end{pmatrix},$$

where $U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and $B = (\boldsymbol{b}_u, \boldsymbol{b}_v)$ with $\boldsymbol{b}_u, \boldsymbol{b}_v \in \{0,1\}^{|V|-2}$ being the incidence vectors of u and v over $V(G_{uv})$.

Consider the eigenvalue equation $\det(\rho I - A(G)) = 0$. Since $\rho > \mu$, the block $\rho I - M$ is positive definite. Applying the Schur complement to the determinant yields

$$\det((\rho I_2 - U) - B^T(\rho I - M)^{-1}B) = 0.$$

Thus, ρ is an eigenvalue of $U + B^T(\rho I - M)^{-1}B$. To show that it is the largest eigenvalue, write the Perron vector of G as $\boldsymbol{x} = (\boldsymbol{x}_{\{u,v\}}^T, \boldsymbol{x}_{V(G_{uv})}^T)^T$. The block eigenvalue equations give

$$\begin{aligned} \boldsymbol{x}_{V(G_{uv})} &= (\rho I - M)^{-1} B \boldsymbol{x}_{\{u,v\}}, \\ \left(U + B^T(\rho I - M)^{-1}B\right) \boldsymbol{x}_{\{u,v\}} &= \rho \boldsymbol{x}_{\{u,v\}}. \end{aligned}$$

The resolvent is entrywise nonnegative by its Neumann series. Hence, the matrix in the second equation is nonnegative and has a strictly positive off-diagonal entry. It is therefore irreducible. Since $\boldsymbol{x}_{\{u,v\}}$ is positive, the Perron–Frobenius theorem implies

$$\rho = \lambda_{\max}\left(U + B^T(\rho I - M)^{-1}B\right).$$

By Lemma 4.3, the resolvent satisfies $(\rho I - M)^{-1} \preceq (\rho I + M)/(\rho^2 - \mu^2)$. Multiplying by B^T and B preserves this partial order, yielding

$$B^T(\rho I - M)^{-1}B \preceq \frac{\rho B^T B + B^T M B}{\rho^2 - \mu^2}.$$

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A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

Since M is a real symmetric matrix and $\lambda_{\max}(M) = \mu$, we have $\mu I - M \succeq 0$, *i.e.*, $M \preceq \mu I$, and therefore, $B^T M B \preceq \mu B^T B$. Substitution gives

$$B^T(\rho I - M)^{-1} B \preceq \frac{\rho B^T B + \mu B^T B}{\rho^2 - \mu^2} = \frac{B^T B}{\rho - \mu}.$$

The 2×2 Gram matrix $B^T B$ is

$$B^T B = \begin{pmatrix} \boldsymbol{b}_u^T \boldsymbol{b}_u & \boldsymbol{b}_u^T \boldsymbol{b}_v \\ \boldsymbol{b}_v^T \boldsymbol{b}_u & \boldsymbol{b}_v^T \boldsymbol{b}_v \end{pmatrix} = \begin{pmatrix} d(u) - 1 & t(e) \\ t(e) & d(v) - 1 \end{pmatrix} := D_e,$$

where $d(u), d(v)$ are the degrees in G, and $t(e)$ is the number of triangles containing e. By Lemma 5.1, we deduce

$$\rho \leq \lambda_{\max}\left(U + \frac{D_e}{\rho - \mu}\right) \leq \lambda_{\max}(U) + \lambda_{\max}\left(\frac{D_e}{\rho - \mu}\right).$$

Noting that $\lambda_{\max}(U) = 1$ and letting $\lambda_D = \lambda_{\max}(D_e)$, we obtain

$$\rho \leq 1 + \frac{\lambda_D}{\rho - \mu}.$$

Since $\rho - \mu > 0$, multiplying both sides by $(\rho - \mu)$ and rearranging terms yield the quadratic inequality $\rho^2 - (\mu+1)\rho + (\mu - \lambda_D) \leq 0$. The discriminant of this quadratic is $\Delta = (\mu+1)^2 - 4(\mu - \lambda_D) = (\mu-1)^2 + 4\lambda_D$, which is nonnegative. Solving for ρ gives the upper bound

$$\rho \leq \frac{1}{2}\left(\mu + 1 + \sqrt{(\mu-1)^2 + 4\lambda_D}\right).$$

Equality in the final bound requires equality throughout the preceding estimates. To track the relevant eigenvector, let $\boldsymbol{z}$ be a positive unit eigenvector of the Schur-complement matrix belonging to ρ. Under equality,

$$\begin{aligned} \rho &= \boldsymbol{z}^T\left(U + B^T(\rho I - M)^{-1}B\right)\boldsymbol{z} \\ &\leq \boldsymbol{z}^T U \boldsymbol{z} + \frac{\boldsymbol{z}^T D_e \boldsymbol{z}}{\rho - \mu} \leq 1 + \frac{\lambda_D}{\rho - \mu} = \rho. \end{aligned}$$

Thus, $\boldsymbol{z}$ attains the largest Rayleigh quotient of both U and D_e and equality holds in the resolvent comparisons evaluated at $B\boldsymbol{z}$.

First, the eigenspace of U belonging to its largest eigenvalue 1 is spanned by $\mathbf{1} = (1,1)^T$. Hence, $\boldsymbol{z} = \mathbf{1}/\sqrt{2}$. Thus, $\mathbf{1}$ is also an eigenvector of D_e belonging to λ_D, so $D_e\mathbf{1} = \lambda_D\mathbf{1}$. This implies $d_G(u) - 1 + t(e) = d_G(v) - 1 + t(e)$, and hence $d_G(u) = d_G(v)$, which establishes condition (i).

Second, the matrix partial order relaxation $B^T(\rho I - M)^{-1}B \preceq \frac{B^T B}{\rho - \mu}$ must achieve equality when evaluated at the principal eigenvector $\mathbf{1}$. This requires the quadratic form to satisfy

$$\mathbf{1}^T\left(B^T(\rho I - M)^{-1}B\right)\mathbf{1} = \mathbf{1}^T\left(\frac{B^T B}{\rho - \mu}\right)\mathbf{1}.$$

Let $\boldsymbol{y} = B\mathbf{1} = \boldsymbol{b}_u + \boldsymbol{b}_v$. The condition simplifies to

$$\boldsymbol{y}^T(\rho I - M)^{-1}\boldsymbol{y} = \frac{\boldsymbol{y}^T\boldsymbol{y}}{\rho - \mu}.$$

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A publication of the International Linear Algebra Society
Volume 42, pp. 819-831, October 2026.

Here, both steps in the resolvent estimate must be equalities:

$$\boldsymbol{y}^T(\rho I - M)^{-1}\boldsymbol{y} \leq \frac{\rho\,\boldsymbol{y}^T\boldsymbol{y} + \boldsymbol{y}^T M\boldsymbol{y}}{\rho^2 - \mu^2} \leq \frac{\boldsymbol{y}^T\boldsymbol{y}}{\rho - \mu}.$$

Lemma 4.3 alone gives only $M^2\boldsymbol{y} = \mu^2\boldsymbol{y}$. Equality in the second inequality also gives $\boldsymbol{y}^T(\mu I - M)\boldsymbol{y} = 0$. Since $\mu I - M$ is positive semidefinite, this is equivalent to $(\mu I - M)\boldsymbol{y} = 0$. Thus, $M\boldsymbol{y} = \mu\boldsymbol{y}$, that is, $M(\boldsymbol{b}_u + \boldsymbol{b}_v) = \mu(\boldsymbol{b}_u + \boldsymbol{b}_v)$. Conversely, this identity gives equality in both resolvent inequalities.

Finally, we translate the algebraic condition $M(\boldsymbol{b}_u + \boldsymbol{b}_v) = \mu(\boldsymbol{b}_u + \boldsymbol{b}_v)$ into the graph-theoretic condition (ii). For any vertex $x \in V(G_{uv})$, the x-th entry of the vector $(\boldsymbol{b}_u + \boldsymbol{b}_v)$ represents exactly $c(x)$, the number of edges connecting x to the set $\{u, v\}$. The x-th row of the matrix equation $M(\boldsymbol{b}_u + \boldsymbol{b}_v) = \mu(\boldsymbol{b}_u + \boldsymbol{b}_v)$ can be expanded as

$$\sum_{y \in V(G_{uv})} M_{x,y} \cdot c(y) = \mu \cdot c(x).$$

Since $M_{x,y} = 1$ if and only if $y \in N_{G_{uv}}(x)$, the summation on the left is exactly the sum of $c(y)$ over all neighbors of x in G_{uv}.

This proves the necessity of condition (ii).

Conversely, suppose that (i) and (ii) hold. With $\boldsymbol{y} = B\mathbf{1}$, condition (ii) gives $M\boldsymbol{y} = \mu\boldsymbol{y}$, and hence $(\rho I - M)^{-1}\boldsymbol{y} = \boldsymbol{y}/(\rho - \mu)$. Condition (i) implies that the nonnegative matrix D_e has equal row sums, so $D_e\mathbf{1} = \lambda_D\mathbf{1}$. Therefore,

$$\left(U + B^T(\rho I - M)^{-1}B\right)\mathbf{1} = \mathbf{1} + \frac{B^TB\mathbf{1}}{\rho - \mu} = \left(1 + \frac{\lambda_D}{\rho - \mu}\right)\mathbf{1}.$$

Since $\mathbf{1}$ is positive, this eigenvalue is the spectral radius of the Schur-complement matrix, which equals ρ. Thus, $\rho = 1 + \lambda_D/(\rho - \mu)$, and the stated upper bound holds with equality. This completes the equality characterization. □

Acknowledgments. The authors would like to thank the referees for their constructive corrections and valuable comments, which have considerably improved the presentation of this paper.

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