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ARTICLE

Eigenvalues and triangles in graphs

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Abstract
Bollobás and Nikiforov (*J. Combin. Theory Ser. B.* **97** (2007) 859–865) conjectured the following. If G is a K_{r+1}-free graph on at least $r+1$ vertices and m edges, then $\lambda_1^2(G)+\lambda_2^2(G) \leqslant (r-1)/r \cdot 2m$, where $\lambda_1(G)$ and $\lambda_2(G)$ are the largest and the second largest eigenvalues of the adjacency matrix $A(G)$, respectively. In this paper we confirm the conjecture in the case $r=2$, by using tools from doubly stochastic matrix theory, and also characterize all families of extremal graphs. Motivated by classic theorems due to Erdős and Nosal respectively, we prove that every non-bipartite graph G of order n and size m contains a triangle if one of the following is true: (i) $\lambda_1(G) \geqslant \sqrt{m-1}$ and $G \neq C_5 \cup (n-5)K_1$, and (ii) $\lambda_1(G) \geqslant \lambda_1(S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}))$ and $G \neq S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil})$, where $S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil})$ is obtained from $K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}$ by subdividing an edge. Both conditions are best possible. We conclude this paper with some open problems.

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1. Introduction

It is well known that spectra of graphs can be used to describe structural properties and parameters of graphs, including cycle structures [17], maximum cuts [2], matchings and factors [8], regularity [24], diameter [10] and expander properties [1]. Recently there has been extensive research in the literature (see [12], [11], [26], [23], [36], [16] and [25]). Referring to spectral extremal graph theory, the bulk of the related work was included in the detailed survey [32]; see references therein.

In this paper we focus on spectral extremal graph theory and mainly investigate the relationship between triangles and eigenvalues of the adjacency matrix of a graph. Throughout this paper, let G be a graph with order $v(G) := n$, size $e(G) := m$ and clique number $\omega(G) := \omega$. Let $A(G)$ be its adjacency matrix. The eigenvalues $\lambda_1(G) := \lambda_1 \geqslant \lambda_2(G) := \lambda_2 \geqslant \cdots \geqslant \lambda_n(G)$ of $A(G)$ are called the *eigenvalues* of G. For all integers $n \geqslant 1$, we set $[n] = \{1, 2, \ldots, n\}$.

The study of bounding the spectral radius of a graph in terms of some parameters has a rich history. Starting from 1985, Brualdi and Hoffman [9] proved that $\lambda_1 \leqslant k-1$ if $m \leqslant \binom{k}{2}$ for some integer $k \geqslant 1$. This result was extended by Stanley [35], who showed that

$$\lambda_1 \leqslant \frac{1}{2}(\sqrt{8m+1}-1).$$

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The bound is best possible for complete graphs (possibly with isolated vertices) but can be further improved for special classes of graphs, such as triangle-free graphs (see Nosal [33]). For further generalizations and related extensions of Stanley's result, see Hong [20], Hong, Shu and Fang [21], Nikiforov [28] and Zhou and Cho [40]. Concerning bounding the spectral radius of a graph in terms of the clique number, Wilf [37] showed that

$$\lambda_1 \leqslant \frac{\omega - 1}{\omega} n.$$

A better inequality,

$$\lambda_1 \leqslant \sqrt{\frac{2(\omega - 1)m}{\omega}},$$

implicitly conjectured by Edwards and Elphick [14], was confirmed by Nikiforov in [28] using a technique of Motzkin and Straus [27]. Later, the extremal graphs when equality holds were characterized in [29]. By the inequality $\lambda_1 \geqslant 2m/n$, one can easily deduce the concise form of Turán's theorem, that is,

$$m \leqslant \frac{\omega - 1}{2\omega} n^2,$$

from Nikiforov's inequality. Therefore Nikiforov's inequality sometimes is called the spectral Turán theorem.

In 2007, Bollobás and Nikiforov [6] posed the following nice conjecture, which is the original motivation for our article.

Conjecture 1.1 **([6, Conjecture 1]).** *Let G be a K_{r+1}-free graph of order at least $r + 1$ with m edges. Then*

$$\lambda_1^2 + \lambda_2^2 \leqslant \frac{r - 1}{r} \cdot 2m.$$

Note that Conjecture 1.1, if true, will improve Nikiforov's inequality. To our knowledge, the conjecture is still open. In this paper we make the first progress on this conjecture. In fact we solve the case $r = 2$ by using tools from doubly stochastic matrix theory, and also characterize all extremal graphs.

Let G be a graph. A 'blow-up' of G is a new graph obtained from G by replacing each vertex $x \in V(G)$ with an independent set I_x, in which, for any two vertices $x, y \in V(G)$, we add all edges between I_x and I_y if $xy \in E(G)$. Let P_n denote a path on n vertices, *i.e.* a path of length $n - 1$. For an integer $k \geqslant 2$, kP_n denotes the disjoint union of k copies of P_n.

Theorem 1.2. *Let G be a triangle-free graph of order at least 3 with m edges. Then*

$$\lambda_1^2 + \lambda_2^2 \leqslant m,$$

where equality holds if and only if G is a blow-up of some member of $\mathcal{G}$ in which

$$\mathcal{G} = \{P_2 \cup K_1, 2P_2 \cup K_1, P_4 \cup K_1, P_5 \cup K_1\}.$$

Recall that a quintessential result in extremal graph theory is Mantel's theorem, which maximizes the number of edges over all triangle-free graphs. We should emphasize that Theorem 1.2 strengthens the spectral strengthening of Mantel's theorem due to Nosal [33], which states that every triangle-free graph G on m edges satisfies $\lambda_1 \leqslant \sqrt{m}$. On the other hand, Mantel's theorem was improved by Erdős (see [7, Ex. 12.2.7]) in the following form: every non-bipartite triangle-free graph of order n and size m satisfies

$$m \leqslant \frac{(n - 1)^2}{4} + 1.$$

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Note that a subdivision of $K_{\lfloor (n-1)/2\rfloor,\lceil (n-1)/2\rceil}$ on one edge shows that the upper bound is tight. In this paper we shall prove spectral versions of Erdős's theorem.

Our two results are as follows.

Theorem 1.3. *Let G be a non-bipartite graph with size m. If* $\lambda_1 \geqslant \sqrt{m-1}$, *then G contains a triangle unless G is a* C_5 *(possibly together with some isolated vertices).*

Theorem 1.4. *Let G be a non-bipartite graph with order n. If*

$$\lambda_1 \geqslant \lambda_1(S(K_{\lfloor (n-1)/2\rfloor,\lceil (n-1)/2\rceil})),$$

where $S(K_{\lfloor (n-1)/2\rfloor,\lceil (n-1)/2\rceil})$ *denotes a subdivision of* $K_{\lfloor (n-1)/2\rfloor,\lceil (n-1)/2\rceil}$ *on one edge, then G contains a triangle unless*

$$G \cong S(K_{\lfloor (n-1)/2\rfloor,\lceil (n-1)/2\rceil}).$$

2. The Bollobás–Nikiforov conjecture for triangle-free graphs

In Section 2 we introduce necessary preliminaries for doubly stochastic matrix theory and then prove Theorem 1.2. For more details on related knowledge, we refer the reader to Zhan [39].

A non-negative square matrix is called *doubly stochastic* if every entry is at least 0 and the sum of the entries in every row and every column is 1, and it is called *doubly substochastic* if the sum of the entries in every row and every column is less than or equal to 1. A square matrix is called a *weak-permutation matrix* if every row and every column has at most one non-zero entry and all the non-zero entries (if any) are 1.

We also use the definition of 'a vector is weakly majorized by the other one' as follows, where we rearrange the components of $x=(x_1,x_2,\ldots,x_n)$, $y=(y_1,y_2,\ldots,y_n)\in\mathbb{R}^n$ in non-increasing order as $x_{[1]}\geqslant x_{[2]}\geqslant\cdots\geqslant x_{[n]}$ and $y_{[1]}\geqslant y_{[2]}\geqslant\cdots\geqslant y_{[n]}$.

Definition 2.1. Let $x=(x_1,x_2,\ldots,x_n)$, $y=(y_1,y_2,\ldots,y_n)\in\mathbb{R}^n$. If

$$\sum_{i=1}^{k} x_{[i]} \leqslant \sum_{i=1}^{k} y_{[i]},\quad k=1,2,\ldots,n,$$

then we say that x is *weakly majorized by* y and denote it by $x\prec_w y$. If

$$x\prec_w y \quad\text{and}\quad \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i,$$

then we say that x is *majorized by* y and denote it by $x\prec y$.

The following lemma is a basic property on a doubly substochastic matrix.

Lemma 2.1 **([39, Lemma 3.24]).** *Let*

$$x, y\in\mathbb{R}^n_+ = \{(z_1,\ldots,z_n)\mid z_i\geqslant 0, 1\leqslant i\leqslant n\}.$$

Then $x\prec_w y$ *if and only if there exists a doubly substochastic matrix A such that* $x=Ay$.

One of the main ingredients in our proof is using the relationship between a doubly (sub)stochastic matrix and a (weak-)permutation matrix.

Lemma 2.2 **([39, Theorem 3.22]).** *Every doubly substochastic matrix is a convex combination of weak-permutation matrices.*

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The following result will play an essential role in our proof of Theorem 1.2, which uses Minkowski's inequality (see [22, p. 8]).

Lemma 2.3 (Minkowski's inequality). *Let $x, y \in \mathbb{R}_+^n$. If $p > 1$, then $\|x + y\|_p \leqslant \|x\|_p + \|y\|_p$. Moreover, if $x, y \in \mathbb{R}_+^n$, $x \neq \theta$ and $y \neq \theta$, where $\theta = (0, 0, \ldots, 0)$, then equality holds if and only if there exists $\alpha > 0$ such that $x = \alpha y$.*

By induction on k (see below), Lemma 2.3 can be extended to a multiple version easily.

Lemma 2.4 (multiple Minkowski's inequality). *Let $k \in \mathbb{Z}$, $k \geqslant 2$ and $x^i \in \mathbb{R}_+^n$, where $i \in [k]$. If $p > 1$, then*

$$\left\| \sum_{i=1}^{k} x^i \right\|_p \leqslant \sum_{i=1}^{k} \|x^i\|_p.$$

Moreover, if $x^i \neq \theta$ for all i, then equality holds if and only if there exists $\alpha_{i,j} > 0$ such that $x^i = \alpha_{i,j} x^j$ for all $i, j \in [n]$ with $i \neq j$.

Theorem 2.1. *Let $x = (x_1, x_2, \ldots, x_n)$, $y = (y_1, y_2, \ldots, y_n) \in \mathbb{R}_+^n$ such that $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$ are in non-increasing order. If $y \prec_w x$, then $\|y\|_p \leqslant \|x\|_p$ for every real number $p > 1$, where equality holds if and only if $x = y$.*

Proof. If $x = \theta$, then $y = \theta$. Now assume $x \neq \theta$. Since $y \prec_w x$, there exists a doubly substochastic matrix A such that $y = Ax$ by Lemma 2.1. By Lemma 2.2, there are s weak-permutation matrices P_i for all $i \in [s]$, such that $A = \sum_{i=1}^{s} a_i P_i$, where $\sum_{i=1}^{s} a_i = 1$, $a_i \geqslant 0$. Without loss of generality, we can assume $a_i > 0$ for all $i \in [s]$. Note that

$$y = Ax = \left(\sum_{i=1}^{s} a_i P_i \right) x = \sum_{i=1}^{s} a_i (P_i x).$$

Therefore

$$\|y\|_p = \left\| \sum_{i=1}^{s} a_i (P_i x) \right\|_p \leqslant \sum_{i=1}^{s} a_i \|P_i x\|_p \leqslant \sum_{i=1}^{s} a_i \|x\|_p = \left(\sum_{i=1}^{s} a_i \right) \cdot \|x\|_p = \|x\|_p.$$

If $x = y$, then obviously $\|x\|_p = \|y\|_p$. If $\|x\|_p = \|y\|_p$, then

$$\left\| \sum_{i=1}^{s} a_i (P_i x) \right\|_p = \sum_{i=1}^{s} a_i \|P_i x\|_p = \sum_{i=1}^{s} a_i \|x\|_p. \tag{2.1}$$

Since $\|P_i x\|_p \leqslant \|x\|_p$, from (2.1), we obtain $\|P_i x\|_p = \|x\|_p > 0$ for all $i \in [s]$, and so $a_i P_i x \neq \theta$ for each i. By Lemma 2.4, the first equality of (2.1) implies that for any pair of distinct integers $i, j \in [s]$, there exists a real number $\alpha_{i,j} > 0$ such that $a_i (P_i x) = \alpha_{i,j} a_j (P_j x)$. By the second equality of (2.1), since each $a_i > 0$, we have $\|P_i x\|_p = \|x\|_p = \|P_j x\|_p$. Then $\alpha_{i,j} \cdot a_j = a_i \neq 0$. Thus $P_i x = P_j x$ and moreover $P_i x = P_1 x$ for each $i \in [s]$. It follows that $y = \sum_{i=1}^{s} a_i (P_i x) = P_1 x$.

Since $y = P_1 x$ and $\|x\|_p = \|y\|_p$, where P_1 is a weak-permutation matrix, we know that $\{y_i\}_{i=1}^n$ is just a rearrangement of elements of $\{x_i\}_{i=1}^n$. As both $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$ are non-increasing sequences, we have $y = x$. The proof is complete. □

For a graph G, the *rank* of G, denoted by rank (G), is defined as the rank of $A(G)$. We need Theorems 3.3 and 4.3 in [34] to characterize the extremal graphs in Theorem 1.2, so we state them as a lemma below.

Lemma 2.5 ([34]). *Let G be a graph with order n. Then we have the following statements.*

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(I) *If* rank $(G)=2$, *then* G *is a blow-up of* $P_2 \cup K_1$.
(II) *If* G *is a bipartite graph with* rank $(G)=4$, *then* G *is a blow-up of* Γ, *where* $\Gamma \in \{2P_2 \cup K_1, P_4 \cup K_1, P_5 \cup K_1\}$.

We shall give a proof of Theorem 1.2. First we define 'the inertia of a graph' as the ordered triple (n^+, n^-, n^0), where n^+, n^- and n^0 are the numbers (counting multiplicities) of positive, negative and zero eigenvalues of the adjacency matrix $A(G)$, respectively.

Proof of Theorem 1.2. Let n be the order of G and let (n^+, n^-, n^0) be the inertia of G. Set $s^+ := \lambda_1^2 + \cdots + \lambda_{n^+}^2$ and $s^- := \lambda_{n-n^-+1}^2 + \cdots + \lambda_n^2$. Since G is triangle-free, we have $G \ncong K_n$, and so $\lambda_2(G) \geqslant 0$ (see Lemma 5 in [19]).

Suppose that $\lambda_1^2 + \lambda_2^2 > m$. Since $s^+ + s^- = 2m$, we have

$$\lambda_1^2 + \lambda_2^2 > \frac{s^+ + s^-}{2},$$

and so

$$\lambda_1^2 + \lambda_2^2 \geqslant 2(\lambda_1^2 + \lambda_2^2) - s^+ > s^- \geqslant 0.$$

Now we construct two n^--vectors x and y such that

$$x = (\lambda_1^2, \lambda_2^2, 0, \ldots, 0)^T \quad \text{and} \quad y = (\lambda_n^2, \lambda_{n-1}^2, \ldots, \lambda_{n-n^-+1}^2)^T.$$

Since $\lambda_1^2 + \lambda_2^2 > s^-$, we have $y \prec_w x$ and $x \neq y$. Set $p = 3/2$. By Theorem 2.1, we have

$$\|x\|_{3/2}^{3/2} > \|y\|_{3/2}^{3/2},$$

that is,

$$\lambda_1^3 + \lambda_2^3 > |\lambda_n|^3 + |\lambda_{n-1}|^3 + \cdots + |\lambda_{n-n^-+1}|^3.$$

This implies that

$$t(G) = \frac{\lambda_1^3 + \lambda_2^3 + \cdots + \lambda_{n^+}^3 + \lambda_{n-n^-+1}^3 + \cdots + \lambda_n^3}{6} \geqslant \frac{\lambda_1^3 + \lambda_2^3 + \lambda_{n-n^-+1}^3 + \cdots + \lambda_n^3}{6} > 0.$$

This gives us a contradiction. Thus we have proved $\lambda_1^2 + \lambda_2^2 \leqslant m$.

If $\lambda_1^2 + \lambda_2^2 = m$, then $\lambda_1^2 + \lambda_2^2 \geqslant s^- \geqslant 0$. It follows that $y \prec_w x$. By Theorem 2.1, we have

$$\|x\|_{3/2}^{3/2} \geqslant \|y\|_{3/2}^{3/2}.$$

Since G is triangle-free, this implies that

$$0 = t(G) = \frac{\lambda_1^3 + \lambda_2^3 + \cdots + \lambda_{n^+}^3 + \lambda_{n-n^-+1}^3 + \cdots + \lambda_n^3}{6} \geqslant \frac{\lambda_1^3 + \lambda_2^3 + \lambda_{n-n^-+1}^3 + \cdots + \lambda_n^3}{6} \geqslant 0.$$

Therefore

$$\lambda_1^3 + \lambda_2^3 = -(\lambda_{n-n^-+1}^3 + \cdots + \lambda_n^3),$$

which implies

$$\|x\|_{3/2}^{3/2} = \|y\|_{3/2}^{3/2}.$$

Again by Theorem 2.1, $x = y$. It follows that $\lambda_1^2 = \lambda_n^2$ and $\lambda_2^2 = \lambda_{n-1}^2$. Thus $\lambda_1 = -\lambda_n$ and $\lambda_2 = -\lambda_{n-1}$. By the trace formula $\sum_{i=1}^n \lambda_i = 0$, we infer that all the remaining eigenvalues are 0. If $\lambda_2 = 0$, then rank $(G) = 2$. By Lemma 2.5 (I), G is a blow-up of $P_2 \cup K_1$. Recall $\lambda_1 = -\lambda_n$, which implies that G is bipartite. If $\lambda_2 \neq 0$, then rank $(G) = 4$. By Lemma 2.5 (II) and the fact that G is bipartite, G is a blow-up of Γ, where Γ is $2P_2 \cup K_1$ or $P_4 \cup K_1$ or $P_5 \cup K_1$. The proof is complete. □

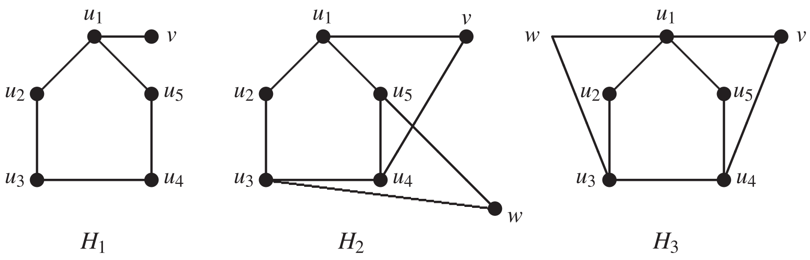

Figure 1. The graphs H_1, H_2 and H_3.

By using the same method as in the proof of Theorem 1.2, we can deduce the following.

Theorem 2.2 **([30, Theorem 2(i)]).** *Let G be a graph of size m. If $\lambda_1^2 \geqslant m$, then G contains a triangle unless G is a blow-up of $P_2 \cup K_1$.*

3. Proofs of Theorems 1.3 and 1.4

A walk $v_1v_2 \cdots v_k$ $(k \geqslant 2)$ in a graph G is called an *internal path* if these k vertices are distinct (except possibly $v_1 = v_k$), $d_G(v_1) \geqslant 3$, $d_G(v_k) \geqslant 3$ and $d_G(v_2) = \cdots = d_G(v_{k-1}) = 2$ (unless $k = 2$). We let G_{uv} denote the graph obtained from G by subdividing the edge uv, *i.e.* introducing a new vertex on the edge uv. Let Y_n be the graph obtained from an induced path $v_1v_2 \cdots v_{n-4}$ by attaching two pendant vertices to v_1 and other two pendant vertices to v_{n-4}.

Hoffman and Smith [18] proved the following result (see also Ex. 14 in [13, p. 79]), which is used towards the structure of extremal graphs in Theorem 1.3.

Lemma 3.1 **([18]).** *Let G be a connected graph with $uv \in E(G)$. If uv belongs to an internal path of G and $G \ncong Y_n$, then $\lambda_1(G_{uv}) < \lambda_1(G)$.*

Now we shall prove Theorems 1.3 and 1.4.

Proof of Theorem 1.3. Suppose to the contrary that G contains no triangles. Assume $\lambda_2 \geqslant 1$. Then $\lambda_1^2 + \lambda_2^2 \geqslant m$. Since G is non-bipartite, by Theorem 1.2, G contains a triangle, a contradiction. Now assume $\lambda_2 < 1$. This implies that if G is disconnected then its every component is an isolated vertex except for one component.

We consider the case that G is connected. Let s be the length of a shortest odd cycle of G, where $s \geqslant 5$. Note that

$$\lambda_2(C_s) = 2\cos\frac{2\pi}{s}.$$

If $s \geqslant 6$, then $\lambda_2(C_s) \geqslant 1$, and by Cauchy's interlacing theorem, $\lambda_2(G) \geqslant \lambda_2(C_s) = 1$, a contradiction. Thus $s = 5$. Let $S = \{u_i \colon 1 \leqslant i \leqslant 5\} \subseteq V(G)$ with $G[S] = u_1u_2u_3u_4u_5u_1$. If $n = 5$, then $G \cong C_5$, and we are done. Let $T = N(S) \backslash S$.

We shall use the property that G contains no H_i as an induced subgraph where $i = 1, 2, 3$, since $\lambda_2(H_i) = 1 > \lambda_2(G)$ (recall H_i in Figure 1). In the following, we say that G is H-free if it contains no H as an induced subgraph.

We first claim that $d_S(v) = 2$ for each $v \in T$. For $v \in T$, without loss of generality, assume that $v \in N(u_1)$. If $d_S(v) \geqslant 3$, then there exists $i \in [5]$ such that $vu_i, vu_{i+1} \in E(G)$, where the subscripts $i, i+1$ are taken modulo 5 and $u_0 = u_5$. In this case there is a triangle $vu_iu_{i+1}v$ in G, a contradiction. If $d_S(v) = 1$, then $N_S(v) = \{u_1\}$ and $\{v, u_1, u_2, u_3, u_4, u_5\}$ induces an H_1, a contradiction. This shows that $d_S(v) = 2$ for each $v \in T$. Next we claim that $V(G) = S \cup T$. Indeed, if not, there exists at least one vertex, say v', which is at distance 2 from S. We can assume that $v'vu_1$ is an induced P_3 such that $v'u_i \notin E(G)$ for any $i \in [5]$. Since $d_S(v) = 2$, by symmetry, we can

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assume $N_S(v) = \{u_1, u_3\}$. Since G is triangle-free and $v'u_i \notin E(G)$ for all $i \in [5]$, we can find that $\{v', v, u_3, u_4, u_5, u_1\}$ induces an H_1, a contradiction. This shows that $V(G) = S \cup T$.

We choose $v \in T$ and assume $N_S(v) = \{u_1, u_3\}$ (by symmetry). Recall that $n \geqslant 6$. If $n = 6$, then $m = 7$, and by a simple calculation, $\lambda_1(G) = 2.3914 < \sqrt{6}$, a contradiction. Therefore $n \geqslant 7$ and this implies $V(G)\backslash(S \cup \{v\}) \neq \emptyset$. It follows that $T\backslash\{v\} \neq \emptyset$.

Let $w \in T\backslash\{v\}$. If $N_S(w) = N_S(v)$ then $wv \notin E(G)$; if $N_S(w) \neq N_S(v)$, then $N_S(w) \cap N_S(v) = \emptyset$, since G is H_3-free and triangle-free. Thus $N_S(w) = \{u_1, u_3\}$, or $N_S(w) = \{u_2, u_4\}$, or $N_S(w) = \{u_2, u_5\}$. Furthermore, for each of the latter two cases, we have $vw \in E(G)$ since G is H_2-free. Indeed, if $N_S(w) = \{u_2, u_4\}$, since G is triangle-free and H_3-free, every vertex in T is adjacent to u_1 and u_3, or to u_2 and u_4; if $N_S(w) = \{u_2, u_5\}$, then every vertex in T is adjacent to u_1 and u_3, or to u_2 and u_5.

In the following we assume $N_S(w) = \{u_2, u_4\}$. Let $A = N_G(u_1) \cap N_G(u_3)$ and $B = N_G(u_2) \cap N_G(u_4)$. By the analysis above, we infer that both A and B are independent sets, $A \cup B = T \cup \{u_2, u_3\}$, and $G[A \cup B]$ is a complete bipartite subgraph. Let $|A| = a$ and $|B| = b$. Then $m = ab + (a+1) + (b+1) = (a+1)(b+1) + 1$, and G is a subdivision of $K_{a+1,b+1}$ on some edge. By Lemma 3.1,

$$\lambda_1(G) < \lambda_1(K_{a+1,b+1}) = \sqrt{(a+1)(b+1)} = \sqrt{m-1},$$

a contradiction.

If G is disconnected, then there is only one non-trivial component. We apply the conclusion obtained above to the component, and we obtain $G = C_5 \cup (n-5)K_1$, where n is the order of G. The proof is complete. □

In the following we use $S(G)$ to denote a subdivision of G on an edge if the subdivision is unique up to isomorphism. The proof of Theorem 1.4 uses two propositions, whose proofs are postponed to the Appendix.

Proposition 3.2. *Let s, t be two integers. If $t \geqslant s \geqslant 1$, then*

$$\lambda_1(S(K_{s+2,t+2})) > \lambda_1(S(K_{s+1,t+3})).$$

Proposition 3.3. *Let s, t be two integers. If $t \geqslant s \geqslant 1$ and $s + t = n - 5$, then*

$$\lambda_1(S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil})) \geqslant \lambda_1(S(K_{s+2,t+2})),$$

where equality holds if and only if

$$(s, t) = (\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil).$$

Proof of Theorem 1.4. Suppose that G is a non-bipartite triangle-free graph of order n with the maximum spectral radius. We will show that

$$G = S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}).$$

First we claim that G is connected, since otherwise we can add a new edge between a component with the maximum spectral radius and any other component to get a new graph with larger spectral radius. We also observe that adding any new edge gives us at least one triangle.

Let $x = (x_1, \ldots, x_n)^t$ be the Perron vector of G and let u be a vertex of G with

$$x_u = \max\{x_i \mid i = 1, \ldots, n\}.$$

Let $C = u_1 u_2 \cdots u_k u_1$ be a shortest odd cycle of G with $k \geqslant 5$. We have the following claims.

Claim 1. *For any two vertices $x, y \in V(G)$, the distance between x and y in G, denoted by $d_G(x, y)$, satisfies that $d_G(x, y) \leqslant 2$.*

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Proof. For any two non-adjacent vertices $x, y \in V(G)$, let $P = v_0v_1v_2 \cdots v_l$ be a shortest (x, y)-path in G, where $v_0 = x$ and $v_l = y$. Obviously $l \geqslant 2$. Since $G + xy$ is not bipartite and $\lambda_1(G + xy) > \lambda_1(G)$, by the choice of G, there is a triangle passing through the edge xy in $G + xy$. That is, there is an (x, y)-path of length 2 in G, and so $d_G(x, y) = 2$. This proves Claim 1. □

Claim 2. $k = 5$.

Proof. Suppose to the contrary that $k \geqslant 7$. Since C is chordless, $u_1u_4 \notin E(G)$. By Claim 1, $d_G(u_1, u_4) = 2$. This means that there exists a vertex outside C, say v, such that u_1vu_4 is a path of length 2. Then $u_1vu_4u_3u_2u_1$ is a cycle of length 5, a contradiction. This proves the claim. □

If $V(C) = V(G)$, then G is an induced 5-cycle, and $G = S(K_{2,2})$. Now assume $V(G)\backslash V(C) \neq \emptyset$ and so $n \geqslant 6$.

Claim 3. *For each vertex* $w \in V(G)\backslash(N(u) \cup V(C))$, $N(w) = N(u)$.

Proof. If $V(G)\backslash(N(u) \cup V(C)) = \emptyset$, then there is nothing to prove. Thus $V(G)\backslash(N(u) \cup V(C)) \neq \emptyset$. Suppose Claim 3 is false. Let $w \in V(G)\backslash(N(u) \cup V(C))$ such that $N(w) \neq N(u)$. Let $G' = G - \{wv \mid v \in N_G(w)\} + \{wv \mid v \in N_G(u)\}$. Obviously G' contains no triangles and C is also in G', and so G' is not bipartite.

Observe that

$$\lambda_1(G') - \lambda_1(G) \geqslant x^t(A(G') - A(G))x \geqslant 2x_w \left(\sum_{v\in N(u)} x_v - \sum_{v\in N(w)} x_v \right) \geqslant 0. \tag{3.1}$$

If $N(w) \subsetneqq N(u)$, then $\lambda_1(G') > \lambda_1(G)$, a contradiction. Therefore

$$N(w)\backslash N(u) \neq \emptyset \quad \text{and} \quad N(u)\backslash N(w) \neq \emptyset.$$

By the choice of G, $\lambda_1(G) \geqslant \lambda_1(G')$. Thus all inequalities of (3.1) become equalities, and so x is also the Perron vector of G'. On the other hand, choosing $z \in N(u)\backslash N(w)$, we have

$$\lambda_1(G)x_z = \sum_{v\in N_G(z)} x_v < \sum_{v\in N_G(z)\cup\{w\}} x_v = \lambda_1(G')x_z,$$

and hence $\lambda_1(G) < \lambda_1(G')$, a contradiction. □

Claim 4. *For any* $s, t \in N(u)\backslash V(C)$, *we have* $N(s) \cap V(C) = N(t) \cap V(C)$.

Proof. Let $w \in N(u)\backslash V(C)$ such that

$$x_w = \max\{x_v \mid v \in N(u)\backslash V(C)\}.$$

Note that $N(u)$ is an independent set. Let

$$Y = \{v \in V(G - C) \mid N(v) = N(u)\}.$$

By Claim 3, we have

$$\lambda_1(G)x_z = \sum_{v\in Y} x_v + \sum_{v\in N(z)\cap V(C)} x_v$$

for any $z \in N(u)\backslash V(C)$. This implies that

$$\sum_{v\in N(w)\cap V(C)} x_v \geqslant \sum_{v\in N(z)\cap V(C)} x_v$$

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for any $z \in N(u)\backslash V(C)$.

If there exists a vertex $z' \in N(u)\backslash V(C)$ such that $N(z') \cap V(C) \neq N(w) \cap V(C)$, let

$$G' = G - \{z'v \mid v \in N(z') \cap V(C)\} + \{z'v \mid v \in N(w) \cap V(C)\}.$$

Then

$$\lambda_1(G') - \lambda_1(G) \geqslant x^t(A(G') - A(G))x \geqslant 2x_j \left(\sum_{v \in N(w) \cap V(C)} x_v - \sum_{v \in N(z') \cap V(C)} x_v \right) \geqslant 0.$$

One can find that G' is connected, non-bipartite and triangle-free. Similarly to the proof of Claim 3, we have $\lambda_1(G') > \lambda_1(G)$, a contradiction. Thus, for any $z \in N(u)\backslash V(C)$, $N(z) \cap V(C) = N(w) \cap V(C)$. This proves Claim 4. □

Let $X = N(u)\backslash V(C)$ and $Y = \{v \in V(G - C) | N(v) = N(u)\}$. From Claim 3, we have $V(G) = X \cup Y \cup V(C)$. In what follows, we only need to consider three cases: (A) $u \notin V(C)$ and $X \neq \emptyset$, (B) $u \notin V(C)$ and $X = \emptyset$, and (C) $u \in V(C)$.

Let us first consider case (A). For this case, $X \neq \emptyset$ and $Y \neq \emptyset$. By Claims 3 and 4, we have $X \cup Y = V(G)\backslash V(C)$, $G - C = B(X, Y) \cong K_{s,t}$, where $|X| = s$, $|Y| = t$, $t \geqslant s \geqslant 1$. Moreover, any two vertices in X have the same neighbour (neighbours) of C, and any two vertices in Y also have the same neighbour (neighbours) of C.

Claim 5. *By symmetry, we have $N_C(X) = \{u_i, u_{i+2}\}$ and $N_C(Y) = \{u_j, u_{j+2}\}$ such that $N_C(X) \cap N_C(Y) = \emptyset$.*

Proof. We first observe that for any vertex $v \in V(G\backslash C)$, $|N(v) \cap V(C)| \leqslant 2$, since G is triangle-free and $|V(C)| = 5$. Next we shall show that $d_C(X) = d_C(Y) = 2$. Since G is connected, we have $d_C(X) \geqslant 1$ or $d_C(Y) \geqslant 1$. Assume that $d_C(X) = 1$ and set $N_C(X) = \{u_i\}$. If either u_{i+2} or u_{i-2} does not belong to $N_C(Y)$, then we connect such a vertex to all vertices in X, and create a new graph G'. Note that G' is non-bipartite and triangle-free but with larger spectral radius, a contradiction. Hence $u_{i+2}, u_{i-2} \in N_C(Y)$. Since C is a 5-cycle, $u_{i-2}u_{i+2} \in E(G)$ and there is a triangle in G, a contradiction. Therefore $d_C(X) = 2$, and by symmetry, $N_C(X) = \{u_i, u_{i+2}\}$. The other assertion can be proved similarly. From the fact that G contains no triangles it follows that $N_C(X) \cap N_C(Y) = \emptyset$. □

By Claim 5 and the symmetry, without loss of generality, we can assume $N_C(X) = \{u_1, u_3\}$ and $N_C(Y) = \{u_2, u_4\}$. By Claim 2, C is an induced 5-cycle. By Claims 3 and 4, all vertices of X are adjacent to $\{u_1, u_3\}$, and all vertices of Y are adjacent to $\{u_2, u_4\}$. Furthermore, u_5 is a vertex of degree 2 in G. Observe that $G = S(K_{s+2,t+2})$. By Proposition 3.3 and the choice of G,

$$G = S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}).$$

This finishes case (A).

Now we consider case (B). For this case, by the fact that G is connected and the choice of G, we have $d_C(u) = 2$. Set $N_C(u) = \{u_1, u_3\}$. By Claim 3, we infer $G = S(K_{n-3,2})$. By Proposition 3.3,

$$\lambda_1(G) = \lambda_1(S(K_{n-3,2})) \leqslant \lambda_1(S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil})),$$

where equality holds if and only if $n = 6$ (recall that $n \geqslant 6$). Thus $G = S(K_{2,3})$, where $n = 6$.

Finally we consider Case (C). By an analysis very similar to that above, one can see that

$$G = S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil}).$$

The proof is complete. □

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4. Concluding remarks

In this paper we consider the Bollobás–Nikiforov conjecture on the largest eigenvalue, the second largest eigenvalue and size of a graph, and settle the conjecture for triangle-free graphs, improving the spectral version of Mantel's theorem. We also prove two spectral analogues of Erdős's theorem. Many intriguing problems with respect to this topic remain open.

(a) One can prove the following extension of Erdős's theorem. Let G be a graph with order n and the length of odd girth at least $2k+3$. If G is non-bipartite, then

$$e(G) \leqslant \left(\frac{n-(2k-1)}{2}\right)^2 + 2k - 1.$$

The following question naturally arises: Which class of graphs can attain the maximum spectral radius among the class of graphs above? From Theorem 1.4 we can see that

$$S(K_{\lfloor (n-1)/2 \rfloor, \lceil (n-1)/2 \rceil})$$

is the answer for this problem when $k=1$.

(b) Nosal [33] proved that every graph G of size m satisfying $\lambda_1(G) > \sqrt{m}$ contains a triangle. Nikiforov [31, Theorem 2] proved that every graph G of size $m \geqslant 9$ contains a C_4 if $\lambda_1(G) > \sqrt{m}$. Let k and m be two integers such that $k|m$ and k is odd. Let $S_{m/k+(k+1)/2,k}$ be the graph obtained by joining each vertex of K_k to

$$\frac{m}{k} - \frac{k-1}{2}$$

isolated vertices. Zhai, Lin and Shu [38] conjectured a more general one.

Conjecture 4.1 **([38]).** *Let G be a graph of sufficiently large size m without isolated vertices and let $k \geqslant 1$ be an integer. If*

$$\lambda_1(G) \geqslant \lambda_1(S_{m/k+(k+1)/2,k}),$$

then G contains C_t for every $t \leqslant 2k+2$ unless

$$G = S_{m/k+(k+1)/2,k}.$$

When $k=1$, it includes Nosal's theorem [33] and Nikiforov's theorem [31, Theorem 2] as two special cases.

(c) By replacing $\lambda_1(G)$ with $s^+(G)$, some spectral graph theorists have refined and generalized many classical results on spectral graph theory. For example, Hong's famous theorem [20] states that $\lambda_1(G) \leqslant \sqrt{2m-n+1}$ holds for all connected graphs G with order n and size m. (In fact it holds for all graphs without isolated vertices.) Elphick, Farber, Goldberg and Wocjan [15] made the following conjecture.

Conjecture 4.2 **([15]).** *Let G be a connected graph of order n. Then*

$$\min\{s^+(G), s^-(G)\} \geqslant n-1.$$

Motivated by Conjecture 4.2, we can reconsider Conjecture 1.1 in a general form.

Problem 4.3. Let H be a given graph and let G be an H-free graph of size m. How do we estimate the upper bound of $s^+(G)$ in terms of H and m?

Even if $H = K_{r+1}$, this problem seems harder than Conjecture 1.1. For graphs with given chromatic number, a related problem was studied by Ando and Lin in [3].

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Appendix A.

In this section we shall prove Proposition 3.2, which implies Proposition 3.3.

Proof of Proposition 3.2. Set $G_1 = S(K_{s+2,t+2})$ and $G_2 = S(K_{s+1,t+3})$. Since both G_1 and G_2 contain C_5 as a proper subgraph, we have $\lambda_1(G_i) > 2$ for $i = 1, 2$. The characteristic polynomial of G_1 is

$$P_{G_1}(x) = x^{s+t}(x^5 - (2s + 2t + st + 5)x^3 + (4s + 4t + 3st + 5)x - 2s - 2t - 2st - 2),$$

where $|V(G_1)| = s + t + 5$. Let

$$f(x, s, t) = x^5 - (2s + 2t + st + 5)x^3 + (4s + 4t + 3st + 5)x - 2s - 2t - 2st - 2.$$

Then $\lambda_1(G_1)$ is the largest root of $f(x, s, t) = 0$. Note that

$$f(x, s - 1, t + 1) - f(x, s, t) = (x - 1)^2(x + 2)(t - s + 1).$$

Since $t \geqslant s$, we have $f(x, s - 1, t + 1) - f(x, s, t) > 0$ when $x > 1$. Moreover, since $\lambda_1(G_2)$ is the largest root of $f(x, s - 1, t + 1) = 0$, it follows that $\lambda_1(G_1) > \lambda_1(G_2)$. □

We also include a proof of the result mentioned in Section 4 here. The proof uses a result due to Andrásfai, Erdős and Sós [4] to control the minimum degree.

Lemma A.1 ([4]). *Let G be a graph with order n and odd girth at least $2k + 1$, where $k \geqslant 1$. If the minimum degree $\delta(G) > 2n/(2k + 1)$, then G is bipartite.*

Theorem A.1. *Let G be a graph with order n and odd girth at least $2k + 3$, where $k \geqslant 1$. If G is non-bipartite, then*

$$e(G) \leqslant \left(\frac{n - (2k - 1)}{2}\right)^2 + 2k - 1.$$

Proof of Theorem A.1. We prove Theorem A.1 by induction on n. If $n = 2k + 3$, then the odd girth is $2k + 3$, and hence $G \cong C_{2k+3}$ and $e(G) = 2k + 3$. The result holds. Now we assume $n \geqslant 2k + 4$ and the result holds for graphs with order less than n.

First suppose

$$\delta(G) > \frac{n - (2k - 1)}{2} - \frac{1}{4},$$

that is,

$$\delta(G) \geqslant \frac{n - (2k - 1)}{2}.$$

Since $n > 2k + 3$, we have $(2k - 1)n > (2k - 1)(2k + 3)$, which implies

$$\frac{n - (2k - 1)}{2} > \frac{2n}{2k + 3}.$$

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By Lemma A.1, G is bipartite, a contradiction. Thus

$$\delta(G) \leqslant \frac{n-(2k-1)}{2} - \frac{1}{4}.$$

Let v be a vertex with $d(v) = \delta(G)$ and let $G' = G - \{v\}$.

If G' is non-bipartite, then by the hypothesis we have

$$e(G') \leqslant \left(\frac{n-1-(2k-1)}{2}\right)^2 + 2k - 1 = \left(\frac{n-(2k-1)}{2}\right)^2 + 2k - 1 - \frac{n-(2k-1)}{2} + \frac{1}{4}.$$

It follows that

$$e(G) \leqslant \left(\frac{n-(2k-1)}{2}\right)^2 + 2k - 1.$$

Thus G' is bipartite. Then every odd cycle passes through v in G. Choose C as a shortest odd cycle of G, where $|C| \geqslant 2k+3$. Let $G' = B(X, Y)$, where (X, Y) is the bipartition of G'. Let $X_0 = X \cap (V(C) - \{v\})$, $Y_0 = Y \cap (V(C) - \{v\})$, $X_1 = X - X_0$ and $Y_1 = Y - Y_0$. Then

$$\begin{aligned} e(G) &= e(G[C]) + |E(C, G[X_1, Y_1])| + |E(G[X_1, Y_1])| \\ &\leqslant |C| + 2|X_1| + 2|Y_1| + |X_1||Y_1| \\ &= |C| + (|X_1| + 2)(|Y_1| + 2) - 4 \\ &\leqslant |C| + \left(\frac{|X_1| + 2 + |Y_1| + 2}{2}\right)^2 - 4 \\ &= |C| + \left(\frac{n - |C| + 4}{2}\right)^2 - 4. \end{aligned}$$

Let

$$f(x) = x + \left(\frac{n-x+4}{2}\right)^2 - 4.$$

Then $f'(x) = 1 - (n - x + 4) = x - (n+3)$. Hence for $2k + 3 \leqslant x \leqslant n$ we have

$$f(x) \leqslant f(2k+3) = \left(\frac{n-(2k-1)}{2}\right)^2 + 2k - 1.$$

The proof is complete. □

Remark A.1. Theorem A.1 may have already appeared in the literature. Since we have not yet found this result elsewhere, we have presented a proof here for completeness.

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