New bounds on the spectral radius of graphs based on the moment problem

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October 2019

Abstract

Let \( G \) be an undirected graph, write \( A \) for its adjacency matrix and \( \rho \) for its spectral radius. Let \( w_k, \phi_k \) and \( \phi_k^\star \) be the number of walks, closed walks and closed walks starting and ending at vertex \( i \), respectively. In this paper we show that \( w_k, \phi_k \) and \( \phi_k^\star \) can be regarded as the moments of measures supported on \([-\rho, \rho]\), and therefore they constrain the possible values of \( \rho \). By using classical results from probability theory, we are able to formulate a hierarchy of new lower and upper bounds on \( \rho \), as well as provide alternative proofs to many well known bounds in the literature.

Keywords: walks on graphs, spectral radius, moment problem

1 Introduction

For an undirected graph \( G = (V, \mathcal{E}) \) with vertex set \( V = \{1, \ldots, n\} \) and edge set \( \mathcal{E} \subset V \times V \), we define a walk of length \( k \), or \( k \)-walk, as a sequence of vertices \((i_0, i_1, \ldots, i_k)\) such that \((i_s, i_{s+1}) \in \mathcal{E}\) for \( s \in \{0, \ldots, k-1\} \). A walk of length \( k \) is called closed if \( i_0 = i_{k-1} \), and if \( i_0 = i_{k-1} = j \), i.e., it starts and ends at vertex \( j \), we call it a closed walk for vertex \( j \). We denote the number of length \( k \) walks, closed walks, and closed walks for vertex \( j \) by \( w_k, \phi_k \), and \( \phi_k^\star \), respectively. Write \( A \) for the adjacency matrix of graph \( G \), and \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \) for the spectrum of \( A \), which we will also refer to as the spectrum of \( G \). Denoting the spectral radius of \( A \) by \( \rho \), we know from Perron-Frobenius’ theorem [9] that \( \rho = \lambda_1 \).

There are several lower bounds on \( \rho \) in the literature, formulated in terms of \( w_k \). Bounds in terms of closed walks are rarer (see, e.g., [13]). Many of these bounds come from dexterous applications of Rayleigh principle or the Cauchy-Schwarz inequality. For example, the bounds

\[
\rho \geq \frac{w_1}{w_0}, \quad \rho^2 \geq \frac{w_2}{w_0}, \quad \rho^2 \geq \frac{w_4}{w_2}, \quad \rho^2 \geq \frac{w_6}{w_4},
\]

(1)

which were discovered by Collatz and Sinogowitz [17], Hoffmeister [7], Yu et. al. [20], and Hong and Zhang [8], respectively, make use of these tools. Nikiforov¹ [11] generalized these results, by

¹Nikiforov’s notation in [11] indexes \( w_k \) in terms of the number of nodes instead of the number of edges.
expressing the number of walks \( w_k \) in terms of the eigenvalues, to obtain bounds of the form

\[
\rho^{r} \geq \frac{w_{2s+r}}{w_{2s}},
\]

(2)

for \( z, r \in \mathbb{N}_0 \). Cioabă and Gregory provide an improvement to the first bound in (1)

\[
\rho \geq \frac{w_1}{w_0} + \frac{1}{w_0(\Delta + 2)},
\]

(3)

where \( \Delta \) is the highest degree amongst nodes in \( G \). Nikiforov [12] showed that

\[
\rho > \frac{w_1}{w_0} + \frac{1}{2w_0 + w_1},
\]

(4)

and Favaron et. al [5] used the fact that there is a \( K_{1,\Delta} \) subgraph in \( G \) to obtain

\[
\rho \geq \sqrt{\Delta}.
\]

(5)

There is a number of upper bounds on \( \rho \) in terms of graph invariants like the domination number [15], chromatic number [3, 4], and clique number [4]. Nikiforov [11] provides a whole hierarchy of bounds in terms of the clique number \( \omega(G) \), which for \( k \in \mathbb{N}_0 \) are given by

\[
\rho^{k+1} \leq \left( 1 - \frac{1}{\omega(G)} \right) w_k.
\]

(6)

Let \( u_1 \) be the principal eigenvector of \( A \). Wilf [19] proved the following upper bound in terms of the fundamental weight, defined as \( \sum_{j=1}^{n} u_{1j} \),

\[
\rho \leq \frac{\omega(G) - 1}{\omega(G)} \left( \sum_{i=1}^{n} u_{i1} \right)^2,
\]

(7)

and Cioaba and Gregory [2] showed that, for \( k \in \mathbb{N}_0 \),

\[
\rho^{k} \leq \sqrt{w_{2k}} \max_{1 \leq j \leq n} u_{1j}.
\]

(8)

Moreover, Van Mieghem [16] discovered the bound

\[
\rho^{k} \leq \frac{w_k}{\sum_{j=1}^{n} u_{1j}} \max_{1 \leq i \leq n} u_{1i}.
\]

(9)

In this paper we provide upper and lower bounds for \( \rho \) by expressing the sequences \( \{w_k\}_{k=0}^{\infty}, \{\phi_k\}_{k=0}^{\infty} \) and \( \{\phi_k^{(i)}\}_{k=0}^{\infty} \) as moments of particular measures supported on \( [-\rho, \rho] \), an idea first explored in [13]. Given this representation, we can make use of classical results from probability theory that relate the moment sequence with constraints on its support. This method can produce new bounds on the spectral radius as well as give alternative proofs to many existing bounds in the literature, thus revealing a rather surprising connection between them.

The rest of the paper is organized as follows. Section 2 outlines the tools we will use to analyze walks on graphs using moment sequences. Section 3 discusses lower bounds on the spectral radius derived from the moment problem, and Section 4 discusses upper bounds.
2 Background and Preliminaries

Throughout this paper we use standard graph theory notation, as in [18]. We will use upper case letters for matrices, calligraphic upper case letters for sets and lower case bold letters for vectors. For vector \( \mathbf{v} \) or matrix \( M \), we denote by \( \mathbf{v}^\top \) and \( M^\top \) their respective transposes. For a matrix \( M \) and a set \( J \subset \mathbb{N} \), the matrix \( M_J \) is defined to be the submatrix of \( M \) where columns and rows with indices not in \( J \) have been removed. \( M_J \) is also called a principal submatrix of \( M \), and if \( J = \{1, \ldots, k\} \) we call it a leading principal submatrix. Finally, we say matrix \( M \in \mathbb{R}^{n \times n} \) is positive semidefinite (resp. positive definite) if for every non-zero vector \( \mathbf{v} \in \mathbb{R}^n \) we have \( \mathbf{v}^\top M \mathbf{v} \geq 0 \) (resp. \( \mathbf{v}^\top M \mathbf{v} > 0 \)) and we denote this with \( M \succeq 0 \) (resp. \( M \succ 0 \)).

2.1 Spectral measures and walks

We can relate walks and closed walks on a graph \( G \) to its spectrum by analyzing particular measures, described in detail below, which are supported on the spectrum whose moments correspond to walks.

We begin by stating the following known result which follows directly from the definition of matrix multiplication, and hence we state without proof.

**Lemma 2.1.** For any integer \( k \), the \((i, j)\)-th entry of the matrix \( A^k \) is equal to the number of \( k \)-walks from vertex \( i \) to vertex \( j \) on graph \( G \).

Since \( G \) is undirected \( A \) is symmetric, hence it admits an orthogonal diagonalization. In particular, let \((u_1, u_2, \ldots, u_n)\) be orthonormal eigenvectors of \( A \) corresponding to the eigenvalues \((\lambda_1, \lambda_2, \ldots, \lambda_n)\), and we have

\[
A^k = U \text{diag} (\lambda_1^k, \ldots, \lambda_n^k) U^\top,
\]

for every \( k \geq 0 \), where \( U := [u_1, u_2, \ldots, u_n] \). From this factorization we can obtain identities which will be used in the following sections.

**Lemma 2.2.** Define \( c^{(i)}_l := u^2_{il} \) and \( c_l := (\sum_{l=1}^n u_{il})^2 \), then for every \( k \geq 0 \) we have

\[
(A^k)_{ij} = \sum_{l=1}^n u_{il} \lambda^k_l u_{jl},
\]

\[
\phi_k = \sum_{i=1}^n (A^k)_{ii} = \sum_{i=1}^n \lambda^k_i,
\]

\[
\phi_k(i) = (A^k)_{ii} = \sum_{l=1}^n c^{(i)}_l \lambda^k_l,
\]

\[
w_k = \sum_{i,j}(A^k)_{ij} = \sum_{l=1}^n c_l \lambda^k_l.
\]

**Proof.** The first equality comes from a direct computation from the diagonalization of \( A \). The remaining identities simply make use of the first identity and the fact that \( \sum_{l=1}^n c^{(i)}_l = 1 \), which holds because \( u_i \) has norm 1.

Next we introduce three atomic measures supported on the spectrum which will be closely related to walks and closed walks.
Definition 2.1 (Spectral measures). Let $\delta(\cdot)$ be the Dirac delta measure. For a simple graph $G$ with eigenvalues $\lambda_1 \geq \lambda_2, \cdots \geq \lambda_n$, define the closed-walks measure as

$$\mu_G(x) := \sum_{i=1}^{n} \delta(x - \lambda_i),$$

the closed-walks measure for vertex $i$ as

$$\mu_i^{(i)}(x) := \sum_{l=1}^{n} c_l^{(i)} \delta(x - \lambda_l),$$

and the walks measure as

$$\nu_G(x) := \sum_{l=1}^{n} c_l \delta(x - \lambda_l).$$

Lemma 2.3. For a real measure $\zeta(x)$, define its $k$-th moment as $E(\zeta(X^k))$. Then, the spectral measures defined in (2.1) satisfy

$$E(\mu_G(X^k)) = \phi_k,$$

$$E(\nu_G(X^k)) = w_k.$$

Proof. For the case of $\mu_G$, we evaluate the expected value

$$E(\mu_G(X^k)) = \int_R x^k d\mu_G = \sum_{i=1}^{n} \lambda_i^k = \phi_k.$$

The other two cases have analogous proofs. □

2.2 The moment problem

In order to derive bounds on the spectral radius $\rho$, we will make use of classical results from probability theory which give solutions to the moment problem. These results give necessary and sufficient conditions for a sequence of real numbers to be the moment sequence of a measure supported on a set $K \subseteq \mathbb{R}$. This definition is formalized below.

Definition 2.2 ($K$-moment sequence). The infinite sequence of real numbers $\mathbf{m} = (m_0, m_1, m_2, \ldots)$ is called a $K$-moment sequence if there exists a Borel measure $\zeta(x)$ supported on $K \subseteq \mathbb{R}$ such that

$$m_k = \int_K x^k d\zeta(x).$$

The following result, known as Hamburger’s theorem [14], will be used in Sections 3 and 4.

Theorem 1 (Hamburger’s theorem [14]). Let $\mathbf{m} = (m_0, m_1, m_2, \ldots)$ be an infinite sequence of real numbers. For $n \in \mathbb{N}_0$, define the Hankel matrix $H_n(\mathbf{m})$ as

$$H_n(\mathbf{m}) := \begin{bmatrix}
m_0 & m_1 & m_2 & \cdots & m_n 
m_1 & m_2 & m_3 & \cdots & m_{n+1} 
m_2 & m_3 & m_4 & \cdots & m_{n+2} 
\vdots & \vdots & \vdots & \ddots & \vdots 
m_n & m_{n+1} & m_{n+2} & \cdots & m_{2n}
\end{bmatrix}.$$
The sequence $m$ is a $R$-moment sequence if and only if for every $n \in \mathbb{N}_0$,

$$H_n(m) \succeq 0.$$  \hspace{1cm} (10)

The characterizations of moment sequences supported on intervals of the form $(-\infty, u]$ and $[-u, u]$ are known as the Stieltjes and Hausdorff moment problems, respectively. A proof for the following theorem is known as Stieltjes’ theorem and can be found in [13] for the case where $u = 0$, but it can be easily adapted to the general case through a simple change of variables.

**Theorem 2** (Stieltjes’ theorem). Let $m = (m_0, m_1, m_2, \ldots)$ be an infinite sequence of real numbers. For $n \in \mathbb{N}_0$, define the Hankel matrix $S_n(m)$ as

$$S_n(m) := \begin{bmatrix}
m_1 & m_2 & m_3 & \cdots & m_{n+1} \\
m_2 & m_3 & m_4 & \cdots & m_{n+2} \\
m_3 & m_4 & m_5 & \cdots & m_{n+3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
m_{n+1} & m_{n+2} & m_{n+3} & \cdots & m_{2n+1}
\end{bmatrix}.$$  

The sequence $m$ is a $(-\infty, u]$-moment sequence if and only if for every $n \in \mathbb{N}_0$,

$$H_n(m) \succeq 0,$$  \hspace{1cm} (10)

$$uH_n(m) - S_n(m) \succeq 0.$$  \hspace{1cm} (11)

Similarly, the sequence $m$ is a $(-u, \infty]$-moment sequence if and only if for every $n \in \mathbb{N}_0$,

$$H_n(m) \succeq 0,$$  \hspace{1cm} (12)

$$uH_n(m) + S_n(m) \succeq 0.$$  \hspace{1cm} (13)

The positive (semi)definiteness in the above theorems can be certified by means of the following result known as Sylvester’s criterion.

**Theorem 3** (Sylvester’s criterion [10]). A matrix $M$ is positive semidefinite if and only if for every leading principal submatrix $H$,

$$\det(H) \geq 0.$$  

Moreover, it is positive definite if and only if for every principal submatrix $H$,

$$\det(H) > 0.$$  

## 3 Lower Bounds on the Spectral Radius

By Perron-Frobenius we know that the spectral measures defined in (2.1) are supported on $[-\rho, \rho]$. This implies that the number of walks, which are the moments of those spectral measures, impose constraints on how small the value of $\rho$ can be. Formally, we make use of Theorem 2 to provide lower bounds on $\rho$, given that there is a measure supported on $[-\rho, \rho]$ whose moments are those of $\mu_{G}, \nu_{G}$ or $\nu_{G}^{(i)}$. This leads to the following result.

**Theorem 4.** For a graph $G$, let $m = \{\phi_s\}_{s=0}^{\infty}$ (resp. $\{w_s\}_{s=0}^{\infty}$, $\{\phi_s(j)\}_{s=0}^{\infty}$ for fixed $j \in \{1, \ldots, n\}$) and let $H(m)$ and $S(m)$ be defined as in Theorem 2. Then, for any finite set $J \subset \mathbb{N}_0$,

$$\rho[H(m)]_J - [S(m)]_J \succeq 0,$$  \hspace{1cm} (14)

$$\rho[H(m)]_J + [S(m)]_J \succeq 0.$$  \hspace{1cm} (15)
Proof. This theorem is a corollary of Theorem 2. Since \( m \) corresponds to the sequence of moments of a measure supported in \([-\rho, \rho]\), it follows that \( \rho \) must satisfy the necessary conditions (11) and (13). Furthermore, every leading principal submatrix of a positive semidefinite matrix is also positive semidefinite by Sylvester’s criterion, hence the matrix inequalities (14) and (15) follow.

As a remark, we note that if we have a truncated sequence of moments \( \{m_j\}_{j \in J} \) available, we can apply Theorem 4 to any of the \(2^{|J|}\) subsets of \( J \) without knowing a priori which one will yield the best bound. To find the best lower bound possible using Theorem 4, we may efficiently solve the following semidefinite program by using interior point methods [11]:

\[
\begin{align*}
\min & \quad u \\
\text{s.t.} & \quad u H_J - S_J \succeq 0, \\
& \quad u H_J + S_J \succeq 0.
\end{align*}
\]

We can adapt Theorem 4 to obtain closed form bounds involving a few moments. The following corollary analyzes the case where \(|J| = 1\).

**Corollary 3.1.** For an undirected graph \( G \), let \( m = \{\phi_s\}_{s=0}^\infty \) (resp. \( \{w_s\}_{s=0}^\infty \), \( \{\phi_s(j)\}_{s=0}^\infty \) for fixed \( j \in \{1, \ldots, n\} \)). Then for every \( s, k \in \mathbb{N}_0 \),

\[
\rho^k \geq \frac{m_{2s+k}}{m_{2s}},
\]

with \( \alpha = 1 \) (resp. \( c_1, c^{(j)}_1 \) for fixed \( j \in \{1, \ldots, n\} \)).

**Proof.** Let \( \zeta(x) \) be an atomic measure supported on \( \{\lambda_1, \lambda_2, \ldots, \lambda_n\} \), defined as \( \zeta(x) := \sum_{i=1}^n z_i \delta(x - \lambda_i) \) and let \( \{m_0, m_1, \ldots\} \) be its moment sequence. For every \( r \in \mathbb{N}_0 \) and even \( q \), we construct the following measure based on \( \zeta(x) \):

\[
\zeta_{q,r}(x) := \sum_{i=1}^n z_i \lambda_i^q \delta(x - \lambda_i^r).
\]

We see that \( \zeta_{q,r}(x) \) is supported on \( \{\lambda_1^r, \lambda_2^r, \ldots, \lambda_n^r\} \), and its moments are given by the sequence \( \{m_q, m_{q+r}, m_{q+2r}, \ldots\} \). We apply Theorem 4 to \( \zeta_{2s,k}(x) \) for \( \zeta(x) = \mu_G \) (resp. \( \mu_G^{(j)}(x) \) for fixed \( j \in \{1, \ldots, n\} \), \( \mu_G(x) \)). We note that measure \( \zeta_{2s,k}(x) \) is supported on \([-\rho^k, \rho^k] \), and thus, setting \( J = \{1\} \) we obtain:

\[
\rho^k \geq \frac{m_{2s+k}}{m_{2s}},
\]

like we wanted.

If we set \( m = \{w_s\}_{s=0}^\infty \), this corollary gives an alternative proof for the lower bounds in [2] proven by Nikiforov [11]. It also generalizes these results to closed walks.

Another interesting example comes from applying Theorem 4 in the case where \(|J| = 2\). Corollary 3.2 below, gives a new lower bound in terms of the largest root of a quadratic polynomial, its proof relies on the following lemma

**Lemma 3.1.** Let \( m = \{\phi_s\}_{s=0}^\infty \) (resp. \( \{w_s\}_{s=0}^\infty \), \( \{\phi_s(j)\}_{s=0}^\infty \) for fixed \( j \in \{1, \ldots, n\} \)) and for \( s, k \geq 0 \) define the following matrices

\[
\begin{align*}
H^{(2s,k)} := \begin{bmatrix} m_{2s} & m_{2s+k} \\ m_{2s+k} & m_{2s+2k} \end{bmatrix}, \\
S^{(2s,k)} := \begin{bmatrix} m_{2s+k} & m_{2s+2k} \\ m_{2s+2k} & m_{2s+3k} \end{bmatrix}
\end{align*}
\]
Whenever \( \det(H^{(2s,k)}) \neq 0 \), we have,
\[
\rho^{2k} \geq \frac{\det(S^{(2s,k)})}{\det(H^{(2s,k)})}.
\]

**Proof.** Let \( \zeta_{2s,k}(x) \) be the measure defined in the proof of Corollary 3.1 for the base measure \( \zeta(x) = \mu_{p}(x) \) (resp. \( \mu_{p}^{(i)}(x), \nu_{p}(x) \)). Recall that this measure is supported on \( [-\rho, \rho] \) and has moment sequence \( \{m_{q}, m_{q+r}, m_{q+2r}, \ldots \} \). Applying Theorem 4 with \( J = \{1,2\} \) we obtain
\[
\rho^{k} H^{(2s,k)} \geq S^{(2s,k)} \geq 0,
\]
for every non-zero \( x \in \mathbb{R}^{2} \). Let \( \xi_{1} \geq \xi_{2} \geq 0 \) be the eigenvalues of \( H^{(2s,k)} \)
\[^{2}\] By Rayleigh principle we have
\[
\frac{x^{T} H^{(2s,k)} x}{x^{T} x} \leq \xi_{1}, \quad \frac{w^{T} H^{(2s,k)} w}{w^{T} w} = \xi_{2},
\]
for every \( x \) and \( w \) corresponding to the second eigenvector of \( H^{(2s,k)} \). Similarly, let \( \gamma_{1} \geq \gamma_{2} \) be the eigenvalues of \( S^{(2s,k)} \), by Perron-Frobenius, we know that \( \gamma_{1} \geq 0 \). If \( \gamma_{2} < 0 \), then \( \det(S^{(2s,k)}) < 0 \) and the inequality (21) is trivial. If instead \( \gamma_{2} \geq 0 \), then
\[
\frac{x^{T} S^{(2s,k)} x}{x^{T} x} \geq \gamma_{2}, \quad \frac{v^{T} S^{(2s,k)} v}{v^{T} v} = \gamma_{1},
\]
for any \( x \) and \( v \) equal to the first eigenvector. We plug vectors \( v \) and \( w \) into (23) to obtain
\[
\rho^{k} \geq \frac{v^{T} S^{(2s,k)} v}{v^{T} v} \geq \frac{\gamma_{1}}{v^{T} H^{(2s,k)} v} \geq \frac{\gamma_{1}}{\xi_{1}},
\]
and multiplying obtain
\[
\rho^{2k} \geq \frac{\gamma_{1} \gamma_{2}}{\xi_{1} \xi_{2}} = \frac{\det(S^{(2s,k)})}{\det(H^{(2s,k)})}.
\]

We are now ready to prove the following corollary.

**Corollary 3.2.** Let \( m = \{\phi_{s}\}_{s=0}^{\infty} \) (resp. \( \{w_{s}\}_{s=0}^{\infty}, \{\phi_{s}(j)\}_{s=0}^{\infty} \) for fixed \( j \in \{1, \ldots, n\} \)), and for \( s, k \in \mathbb{N}_{0} \), let \( H^{(2s,k)} \) and \( S^{(2s,k)} \) be defined as in Lemma 3.1. Then \( \rho^{k} \) is lower bounded by the largest root of
\[
\det(H^{(2s,k)}) r^{2} - \det(H^{(2s,k)}) r^{2} - m_{2s+k} m_{2s+2k} - m_{2s} m_{2s+3k} \geq 0.
\]
Proof. From inequality (22) we obtain \( \det \left( \rho^k H^{(2s,k)} \pm S_J \right) \geq 0 \), which can be simplified to
\[
\det \left( H^{(2s,k)} \right) \rho^{2k} - |m_{2s+k}m_{2s+2k} - m_{2s}m_{2s+3k}| \rho^k + \det \left( S_J^{(2s,k)} \right) \geq 0.
\]
(26)
If \( \det \left( H^{(2s,k)} \right) = 0 \), the result follows. Otherwise, by Theorem 1 we must have \( \det \left( H^{(2s,k)} \right) > 0 \), and using Lemma (3.1) we know \( \det \left( S_J^{(2s,k)} \right) \leq \det \left( H^{(2s,k)} \right) \rho^{2k} \), which substituting into (26) yields
\[
2 \det \left( H^{(2s,k)} \right) \rho^{2k} - |m_{2s+k}m_{2s+2k} - m_{2s}m_{2s+3k}| \rho^k \geq 0,
\]
and because \( \rho \geq 0 \), we conclude that
\[
\rho^k \geq \frac{|m_{2s+k}m_{2s+2k} - m_{2s}m_{2s+3k}|}{2 \det \left( H^{(2s,k)} \right)}
\]
which is in turn larger than the smallest root of (25). Since the quadratic (25) has positive leading coefficient, (26) implies that \( \rho \) is larger than the largest root of (25).

We can apply Corollary 3.2 with \( s = 0 \) and \( k = 1 \) to the closed-walks measure of a graph \( G \), leveraging the fact that \( \phi_0 = n \) and \( \phi_1 = 0 \), to obtain the following bounds.

**Corollary 3.3.** For graph \( G \) with \( n \) vertices, \( e \) edges and \( T \) triangles
\[
\rho \geq \frac{\phi_3}{2\phi_2} + \sqrt{\left( \frac{\phi_3}{2\phi_2} \right)^2 + \frac{\phi_2}{\phi_0} \left( \frac{3T}{2e} + \sqrt{\left( \frac{3T}{2e} \right)^2 + \frac{2e}{n}} \right)}.
\]
Similarly, because \( \phi_0^{(i)} = 1 \) and \( \phi_1^{(i)} = 0 \) we have

**Corollary 3.4.** For graph \( G \) with \( d_i \) the degree of vertex \( i \) and \( T_i \) the number of triangles including vertex \( i \), we have
\[
\rho \geq \max_{i \in 1, \ldots, n} \frac{\phi_3^{(i)}}{2\phi_2^{(i)}} + \sqrt{\left( \frac{\phi_3^{(i)}}{2\phi_2^{(i)}} \right)^2 + 4 \left( \frac{\phi_2^{(i)}}{\phi_0^{(i)}} \right)^3} = \max_{i \in 1, \ldots, n} \frac{T_i + \sqrt{T_i^2 + d_i^3}}{d_i}.
\]
Notice how Corollary 3.4 implies
\[
\rho \geq T_\Delta + \sqrt{T_\Delta^2 + \Delta^3} \geq \sqrt{\Delta},
\]
where \( \Delta \) is the maximum degree and \( T_\Delta \) is the maximum number of triangles containing one of the vertices of degree \( \Delta \), improving the bound given in (3).

## 4 Upper bounds on the spectral radius

In this section we make use of Theorems 1 and 2 to derive upper bounds on \( \rho \). If we subtract the term corresponding to \( \lambda_1 \) from the measures defined in (2.1), we obtain measures supported on the set \( \{ \lambda_2, \lambda_3, \ldots, \lambda_n \} \subset [-\rho, \rho] \), whose moments are given by
\[
\sum_{i=2}^{n} \lambda_i^k = \phi_k - \rho^k,
\]
(27)
\[ \sum_{i=2}^{n} c_i^j \lambda_i^k = \phi_k(j) - c_1^j \rho^k, \quad (28) \]
\[ \sum_{i=2}^{n} c_1 \lambda_i^k = w_k - c_1 \rho^k. \quad (29) \]

By applying Hamburger’s theorem to these measures we obtain the following theorem.

**Theorem 5.** Let \( m = \{\phi_s\}_{s=0}^{\infty} \) (resp. \( \{w_s\}_{s=0}^{\infty}, \{\phi_s(j)\}_{s=0}^{\infty} \) for fixed \( j \in \{1, \ldots, n\} \)), let \( H(m) \) and \( S(m) \) be defined as in Theorem 4, and define the infinite dimensional Hankel matrix

\[ P := \begin{bmatrix} 1 & \rho & \rho^2 & \cdots \\ \rho & \rho^2 & \rho^3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \]

For any finite \( J \subset \mathbb{N}_0 \),

\[ H(m)_J = \alpha P_J \succeq 0, \quad (30) \]

with \( \alpha = 1 \) (resp. \( c_1, c_1^j \) for fixed \( j \in \{1, \ldots, n\} \)).

**Proof.** We simply note that the matrix \( H(m) - \alpha P \) is the Hankel matrix containing the moments given in (27) (resp. (28), (29)) and the result follows from Theorem 4 and Sylvester’s criterion. \( \square \)

**Corollary 4.1.** Let \( m = \{\phi_s\}_{s=0}^{\infty} \) (resp. \( \{w_s\}_{s=0}^{\infty}, \{\phi_s(j)\}_{s=0}^{\infty} \) for fixed \( j \in \{1, \ldots, n\} \)), then

\[ \rho^2 k \leq \frac{1}{\alpha} m_{2k}, \quad (31) \]

with \( \alpha = 1 \) (resp. \( c_1, c_1^j \) for fixed \( j \in \{1, \ldots, n\} \)).

**Proof.** For \( J = \{k+1\} \) Theorem 5 implies

\[ m_{2k} - \alpha \rho^{2k} \geq 0. \]

This finishes the proof. \( \square \)

We can show that the upper bound obtained from Corollary 4.1 in the case of \( m = \{w_s\}_{s=1}^{\infty} \) tighter that the bound (6) given by Nikiforov [11] (albeit only for even exponents). Rearranging Wilf’s inequality (7), we obtain

\[ \left( 1 - \frac{1}{\omega(G)} \right) \leq \frac{\rho}{c_1}. \quad (32) \]

Moreover, the upper bound (6) can be expressed as

\[ \left( \left( 1 - \frac{1}{\omega(G)} \right) w_{2k} \right)^{\frac{1}{2k+1}}, \]

and by substituting (32) into this upper bound, we obtain

\[ \left( \left( 1 - \frac{1}{\omega(G)} \right) w_{2k} \right)^{\frac{1}{2k+1}} \geq \left( \frac{w_{2k}}{e_1} \right)^{\frac{1}{2k+1}} \]
\[
\left( \frac{w^{2k}}{c_1} \right)^{k+1} = 1,
\]

which is the upper bound from Corollary 4.1.

Using Theorem 5 with larger principal submatrices, we can improve these bounds further. The following original upper bound is obtained by analyzing the case of \( J = \{1, k+1\} \).

**Corollary 4.2.** Let \( m = \{\phi_s\}_{s=0}^\infty \) (resp. \( \{w_s\}_{s=0}^\infty \), \( \{\phi_s(j)\}_{s=0}^\infty \) for \( j \in \{1, \ldots, n\} \)), then

\[
\rho^k \leq \frac{m_k + \sqrt{(\frac{m_0}{\alpha} - 1) (m_0 m_{2k} - m_k^2)}}{m_0}, \tag{33}
\]

where \( \alpha = 1 \) (resp. \( c_1, c_1^{(j)} \), \( j \in \{1, \ldots, n\} \)). Furthermore, these bounds are tighter than those in Corollary 4.1.

**Proof.** Applying Theorem 5 with \( J = \{1, k+1\} \), we conclude that

\[
\det(H(m)_J - \alpha P_J) \geq 0,
\]

which simplifies to the following expression

\[
-m_0 \rho^{2k} + 2m_k \rho^k + \frac{1}{\alpha} (m_0 - \alpha) m_{2k} - m_k^2 \geq 0.
\]

Making the substitution \( y = \rho^k \), we obtain the following quadratic inequality

\[
-m_0 y^2 + 2m_k y + \frac{1}{\alpha} (m_0 - \alpha) m_{2k} - m_k^2 \geq 0.
\]

The quadratic on the left hand side has a negative leading coefficient, which implies it is negative whenever \( y \) is larger than its largest root, which is given by the right hand side of (33). After substituting back \( \rho^k \), the result follows. To see that these bounds improve the ones in Corollary 4.1 note that Corollary 4.1 and (19) imply

\[
m_{2k} \geq \alpha \rho^{2k} \geq \frac{\alpha m_{4k}}{m_{2k}}
\]

\[
\Rightarrow m_{4k} \leq \frac{1}{\alpha} m_{2k}^2
\]

\[
\Rightarrow m_0 m_{4k} - m_{2k}^2 \leq \left( \frac{m_0}{\alpha} - 1 \right) m_{2k}^2,
\]

and we can use the last inequality in (33) to obtain

\[
\rho^{2k} \leq \frac{m_{2k} + \sqrt{(\frac{m_0}{\alpha} - 1) (m_0 m_{4k} - m_{2k}^2)}}{m_0} \leq \frac{m_{2k} + \sqrt{(\frac{m_0}{\alpha} - 1) (\frac{m_0}{\alpha} - 1) m_{2k}^2}}{m_0} = \frac{m_{2k}}{\alpha}.
\]

\[\blacksquare\]
We can apply Corollary 4.2 to the closed-walks measure for node \( i \) with \( \mathcal{J} = \{1, 2\} \) and noting that \( \phi_0(j) = 1 \) and \( \phi_1(j) = 0 \) to obtain the following upper bound.

**Corollary 4.3.** For a graph \( \mathcal{G} \)

\[
\rho^2 \leq \left( \frac{1}{e_1^J} - 1 \right) \phi_2(j) = \left( \frac{1}{x_j^2} - 1 \right) d_j. \tag{34}
\]

where \( d_j \) is the degree of vertex and \( x_j \) is the \( j \)-th component of the principal eigenvector.

Inequality (34) can be written as

\[
x_j \leq \frac{1}{\sqrt{1 + \rho^2 d_j}},
\]

which was first proven by Cioabă and Gregory in \[2\]. Our method provides an alternative proof.

The special case of bipartite graphs allows us to cut the upper bounds in Corollary 4.1 in half for the case of closed walks.

**Corollary 4.4.** For a bipartite graph \( \mathcal{G} \) and \( k \) even

\[
\rho^{2k} \leq \phi_{2k},
\]

\[
\rho^{2k} \leq \frac{\phi_{2k}(i)}{2c_1(i)}.
\]

**Proof.** The symmetry of the spectrum of bipartite graphs implies that if \( \mathcal{G} \) is bipartite then \( \phi_k = \phi_k(j) = 0 \) for odd \( k \). This allows us to construct new measures from the ones in Definition 2.1 whose moments are the even closed walks (resp. closed walks for node \( i \)). These measures are

\[
\tilde{\mu}_G(x) = \sum_{i=1}^{[n/2]} 2\delta \left( x - \lambda_i^2 \right),
\]

\[
\tilde{\mu}_G^{(j)}(x) = \sum_{i=1}^{[n/2]} 2c_1^{(j)} \delta \left( x - \lambda_i^2 \right),
\]

then for every \( k \geq 0 \), Lemma 2.2 implies

\[
\phi_{2k} = \sum_{i=1}^{[n/2]} 2\lambda_i^{2k} = E_{\tilde{\mu}_G} \left( X^k \right),
\]

\[
\phi_{2k}^{(j)} = \sum_{i=1}^{[n/2]} 2c_1^{(j)} \lambda_i^{2k} = E_{\tilde{\mu}_G^{(j)}} \left( X^k \right),
\]

where we used the fact that the components of eigenvectors corresponding to pairs of eigenvalues that are the reflection of one another, are the same up to a sign. The result then follows by adapting the proof of Corollary 4.1 to the measures \( \tilde{\mu}_G(x) \) and \( \tilde{\mu}_G^{(j)}(x) \). \[\square\]

A more general version of Corollary 4.2 is given in the following theorem.
Theorem 6. Define the infinite dimensional Hankel matrix

\[ R := \begin{bmatrix} 1 & r & r^2 & \cdots \\ r & r^2 & r^3 & \cdots \\ r^2 & r^3 & r^4 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}. \]

Let \( m = \{ \phi_s \}_{s=0}^{\infty} \) (resp. \( \{ w_s \}_{s=0}^{\infty}, \{ \phi_s(j) \}_{s=0}^{\infty} \) for \( j \in \{ 1, \ldots, n \} \)), let \( J = \{ j_1, j_2, \ldots, j_n \} \) and let \( J' = \{ j_1, j_2, \ldots, j_{n-1} \} \) for \( j_1, \ldots, j_n \in \mathbb{N} \). Define the following polynomial

\[ Q(r) := \det (H(m)_J - \alpha R_J), \]

where \( \alpha = 1 \) (resp. \( c_1, c_1^{(j)} \) for \( j \in \{ 1, \ldots, n \} \)). If \( J' \) is such that \( H(m)_{J'} \succ 0 \), then

\[ \rho \leq r^*, \]

where \( r^* \) is the largest root of \( Q(r) \).

Proof. We will prove that \( Q(r) \) has a negative leading coefficient equal to \( -\alpha \det (H(m)_{J'}) \). It is well known (see for example [6]) that if \( A \in \mathbb{R}^{n \times n} \) and \( B := uv^T \) is a rank 1 matrix in \( \mathbb{R}^{n \times n} \) then

\[ \det(A + B) = \det(A) + v^T \text{adj}(A)u, \tag{35} \]

where \( \text{adj}(A) \) is the cofactor matrix of matrix \( A \). In order to apply this result, note that

\[ -\alpha R_J = (\alpha (r^{j_1-1}, \ldots, r^{j_n-1}))^T \cdot (-r^{j_1-1}, \ldots, r^{j_n-1}) := (\alpha r)(-r)^T, \]

so applying (35) we obtain

\[ \det(H(m)_J - \alpha R_J) = \det(H(m)_J) - \alpha r^T \text{adj}(H(m)_J)r. \tag{36} \]

It follows that the leading term of \( Q(r) \) will be \( -\alpha C_{s,s} r^{2(j_s-1)} = -\alpha \det(H(J')) < 0 \). By Theorem 4 we have \( Q(\rho) \geq 0 \), and therefore \( \rho \leq r^* \).

Theorem 6 was derived from applying Hamburger’s theorem to the moment sequence \( \{ m_s - \alpha r^s \}_{s=0}^{\infty} \). We can also apply Stieltjes’ theorem to the same moment sequence to obtain a different hierarchy of upper bounds. This is stated in the following theorem.

Theorem 7. Let \( m = \{ \phi_s \}_{s=1}^{\infty} \) (resp. \( \{ w_s \}_{s=0}^{\infty}, \{ \phi_s(j) \}_{s=0}^{\infty} \) for fixed \( j \in \{ 1, \ldots, n \} \)), then for any \( J \in \mathbb{N}_0 \nabla \)

\[ \rho (H(m)_J - \alpha P_J) + (S(m)_J - \alpha P_J) \succeq 0, \tag{37} \]

with \( \alpha = 1 \) (resp. \( c_1, c_1^{(j)} \) for fixed \( j \in \{ 1, \ldots, n \} \)).

Proof. Recall that the moment sequences \( \{ m_s - \alpha r^s \}_{s=0}^{\infty} \) given in (24), (28) and (29) are supported on \( [-\rho, \rho] \) and therefore, by Theorem 2 the result follows.

Theorem 7 can be used to obtain bounds that improve on those of Corollary 4.1. We have the following.
Corollary 4.5. Let \( m = \{ \phi_s \}_{s=0}^{\infty} \) (resp. \( \{ w_s \}_{s=0}^{\infty}, \{ \phi_s(j) \}_{s=0}^{\infty} \) for fixed \( j \in \{1, \ldots, n\} \)) and define the following polynomial

\[
Q(r) := m_{2k}r + m_{2k+1} - 2\alpha r^{2k+1},
\]

where \( \alpha = 1 \) (resp. \( c_1, c_1^{(j)} \) for \( j \in \{1, \ldots, n\} \)). Then

\[
\rho \leq r^*,
\]

where \( r^* \) is the largest root of \( Q(r) \). Furthermore, these bounds are an improvement over the bounds in Corollary 4.1.

Proof. Applying Theorem 7 to \( J = \{ k + 1 \} \) we get

\[
\rho [m_{2k}] + [m_{2k+1}] - 2\alpha \rho [\rho^{2k}] \geq 0
\]

\[
\implies m_{2k} + m_{2k+1} - 2\alpha \rho^{2k+1} \geq 0,
\]

and thus \( Q(\rho) \geq 0 \), since the leading coefficient of \( Q(r) \) is negative, it follows that \( \rho \leq r^* \). To see that this \( r^* = \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} \), we first prove that \( r^* \) is the unique root of \( Q(r) \) in the region defined by

\[
r \geq \left( \frac{m_{2k}}{2\alpha(2k+1)} \right)^{1/2k}. \tag{38}
\]

This is indeed the case because the derivative of \( Q(r) \) is given by

\[
Q'(r) = m_{2k} - 2(2k+1)\alpha r^{2k+1},
\]

which is negative in the interval defined in (38). Also, note that

\[
\left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} \geq \left( \frac{m_{2k}}{2\alpha(2k+1)} \right)^{1/2k}.
\]

Therefore, it suffices to show that

\[
Q \left( \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} \right) \leq 0.
\]

To this end, we evaluate and obtain

\[
Q \left( \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} \right) \leq 0
\]

\[
\iff \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} m_{2k} + m_{2k+1} - 2\alpha \left( \frac{1}{\alpha} m_{2k} \right)^{2k+1} \leq 0
\]

\[
\iff \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} m_{2k} + m_{2k+1} - 2m_{2k} \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k} \leq 0
\]

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\[ \iff \frac{m_{2k+1}}{m_{2k}} \leq \left( \frac{1}{\alpha} m_{2k} \right)^{1/2k}, \]

and the last inequality is true since the left hand side is a lower bound of \( \rho \) by Corollary 4.1 and the right hand side is an upper bound of \( \rho \) by Corollary 4.4. This finishes the proof.

The implicit bound in Corollary 4.5 when applied to the moment sequence \( m = \{ w_s \}_{s=1}^{\infty} \) provides an improvement on the bound given in (3.1) and consequently on the bound (2). By using inequality (7) we can also obtain a bound in terms of the clique number instead of the fundamental weight, which also improves on (2).

**Corollary 4.6.** Define the following polynomial
\[
Q(r) := rm_{2k} + m_{2k+1} - 2 \frac{\omega(G)}{\omega(G)} r^{2k+2},
\]
then
\[ \rho \leq r^*, \]
where \( r^* \) be its largest root of \( Q(r) \). Furthermore this bound is an improvement on the one given in (6).

**Proof.** The proof is very similar to that of Corollary 4.5 after using (7) to show that
\[
\rho w_{2k} + w_{2k+1} = \frac{\omega(G)}{\omega(G)} \rho^{2k+1} \geq \rho w_{2k} + w_{2k+1} - 2\alpha \rho^{2k+1} \geq 0,
\]
and we omit the details.

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