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BOUNDS ON THE SPECTRAL RADIUS OF DIGRAPHS FROM SUBGRAPH COUNTS*

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Abstract. The spectral radius of a directed graph is a metric that can only be computed when the structure of the network is completely known. However, in many practical scenarios, it is not possible to exactly retrieve the whole structure of the network; hence, the exact value of the spectral radius is not computable. Even in these scenarios, it is typically possible to extract local structural properties of a network using, for example, graph crawlers. In this paper, we develop a novel measure-theoretic framework to upper and lower bound the spectral radius of a directed graph using local structural information, in particular, using the counts of a collection of small subgraphs or motifs. Our framework is based on recent results relating the multivariate moment problem with semidefinite programming. Using these results, we develop a hierarchy of (small) semidefinite programs whose solutions provide upper and lower bounds on the spectral radius of a directed graph using, solely, subgraph and motif counts. We numerically validate the quality of our bounds using both random and real-world directed graphs.

Key words. directed graph, spectral radius, moment problem, semidefinite programming

AMS subject classifications. 05C20, 15A18, 15B48, 44A60, 90C22

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1. Introduction.

The underlying structure of many natural and artificial systems often consists of a large number of components interconnected via a complex pattern of connections [1, 2, 3]. Examples of such complex systems include biological [4, 5], brain [6, 7, 8], social [9, 10, 11, 12], and communication [13, 14, 15] networks, to mention a few. In particular, the pattern of interconnections among these components affects the global behavior of the overall system. In this direction, graph theory provides powerful tools to characterize and analyze the structure and function of complex networked systems (see, for example, [1] and the references therein). A common approach to modeling complex networks is via synthetic random models, such as the Erdős–Rényi random graph [16], the Watts–Strogatz small-world model [17], or the Barabási–Albert model [18], among many others [13]. Existing synthetic models have been used to analyze, for instance, the behavior of many networked dynamical processes, such as synchronization of coupled oscillators, network diffusion, or stochastic spreading processes on networks (see [19] and the references therein for a thorough exposition). A fruitful path to analyze the dynamics of networked processes exploits the connection between network eigenvalues and dynamics. For example, the eigenvalues of the Laplacian matrix have a direct influence on network synchronization [20], whereas the eigenvalues of the adjacency matrix can be used to characterize the speed of spreading of epidemic processes in networks [21, 22, 23].

Even though network eigenvalues are of utmost importance, its computation in large-scale networks is a very challenging problem [24]. On the one hand, the sheer

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size of real-world networks makes this problem computationally challenging. On the other hand, it is typically impossible to retrieve the whole structure of many real networks due to privacy and/or security constraints. In contrast, it is usually feasible to extract local samples of the network structure in the form of ego-networks [25] or subgraph counts [5, 26, 27, 28] using graph crawlers. It is, therefore, of interest to analyze the role of local structural samples on the global eigenvalue spectrum of a complex network.

We find in the literature many works aiming to upper and lower bound the spectral radius of a graph from local structural information [29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40]. In [29] and [30], the authors derived an upper bound on the spectral radius of a matrix from its symmetric and skew-symmetric components. Merikoski and Virtanen [33] provided bounds on the sum of selected eigenvalues using the trace and the determinant. Instead of bounding the eigenvalues of arbitrary square matrices, the works [31, 32, 36] provide lower bounds on the spectral radius of general nonnegative matrices. Most of these bounds are based on the traces of the matrix and/or its second power. In [34], the authors use the traces of even-order powers of a matrix to provide upper bounds on the spectral radius of matrices with real spectrums. In [38], the authors obtained lower bounds on the spectral radius of both real and complex matrices using trace information. In [39, 40], the authors bound the spectral radius of an *undirected* graph using subgraph counts. Similar results were obtained for the spectral gap of the Laplacian matrix in [41, 42].

In this paper, we develop a measure-theoretic framework to obtain upper and lower bounds on the spectral radius of large *directed* graphs using counts of small subgraphs. More specifically, by exploiting recent results in the multidimensional moment problem [43], we propose a hierarchy of small semidefinite programs [44] providing converging sequences of upper and lower bounds on the spectral radius. We numerically show that our framework provides accurate upper and lower bounds in real-world directed networks, as well as random synthetic digraphs.

The rest of the paper is organized as follows. In section 2, we introduce certain notions from algebraic graph theory used in our derivations. In section 3, we relate the subgraph counts of a directed graph with the number of closed walks (subsection 3.1), as well as the so-called spectral moments (subsection 3.2). We then introduce the truncated K-moment problem from functional analysis (subsection 3.3), which we then use to lower and upper bound the spectral radius (subsections 3.4 and 3.5, respectively). Furthermore, in section 4, we propose a refined approach to find more accurate bounds on the spectral radius by analyzing the skew-symmetric part of the adjacency matrix. We numerically validate the quality of our bounds using randomly generated directed graphs, as well as real networks in section 5. We conclude our paper in section 6.

2. Notation and preliminaries. Throughout the paper, we use bold and uppercase letters to represent vectors and matrices, respectively. For a (real or complex) vector $\mathbf{x}$, we denote its ith element and 1-norm as x_i and $|\mathbf{x}| = \sum_{i=1}^n |x_i|$, respectively. The cardinality of a set $\mathcal{S}$ is denoted by $|\mathcal{S}|$. We denote by $[n]$ the set of integers from 1 to n. Given nonnegative integers r and n, we define $\mathbb{N}_r^n = \{\mathbf{x} \in \mathbb{N}^n : |\mathbf{x}| \le r\}$. We use $M \succeq 0$ to indicate that a symmetric matrix M is positive semidefinite.

Let $G = (\mathcal{V}, \mathcal{E})$ be a directed graph (digraph) with vertex-set $\mathcal{V} = [n]$ and edge-set $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$. The *order* of a graph is defined as the number of its vertices. A graph G is said to be *undirected* if $(i, j) \in \mathcal{E}$ implies $(j, i) \in \mathcal{E}$ for all $i, j \in \mathcal{V}$. The *out-neighborhood* of vertex $i \in \mathcal{V}$ is defined as $\mathcal{N}_i^+ = \{j \in \mathcal{V} \colon (i, j) \in \mathcal{E}\}$. Similarly, we define the *in-neighborhood* of vertex i as $\mathcal{N}_i^- = \{j \in \mathcal{V} \colon (j,i) \in \mathcal{E}\}$. A *walk* of length k in G is defined as an ordered sequence of vertices $(i_0, i_1, \ldots, i_k)$ with $(i_\ell, i_{\ell+1}) \in \mathcal{E}$ for all $\ell = 0, \ldots, k-1$. When the vertices in the walk are distinct, then we call the walk a *path*. If $i_0 = i_k$, the walk is said to be *closed*; otherwise, the walk is said to be *open*. We say that a vertex $i \in \mathcal{V}$ has a *self-loop* if $(i,i) \in \mathcal{E}$. A graph contains a *multiedge* if there is any directed edge appearing more than once in $\mathcal{E}$. A digraph is said to be *simple* if the digraph does not have self-loops or multiedges. In the rest of the paper, we assume that the digraph under consideration is simple. We say that $G_s = (\mathcal{V}_s, \mathcal{E}_s)$ is a *subgraph* of G, denoted by $G_s \subseteq G$, if $\mathcal{V}_s \subseteq \mathcal{V}$ and $\mathcal{E}_s \subseteq \mathcal{V}_s \times \mathcal{V}_s$ satisfies $\mathcal{E}_s \subseteq \mathcal{E}$. A subgraph G_s is a *bidirected edge* if $\mathcal{V}_s = \{i,j\}$ and $\mathcal{E}_s = \{(i,j),(j,i)\}$, where $i,j \in \mathcal{V}$. A subgraph G_s is a *directed triangle* if $\mathcal{V}_s = \{i,j,k\}$ and $\mathcal{E}_s = \{(i,j),(j,k),(k,i)$, where $i,j,k \in \mathcal{V}\}$.

A digraph G can be represented by an *adjacency matrix* $A \in \mathbb{R}^{n\times n}$, whose entries are defined as $[A]_{ij} = 1$ if $(j,i) \in \mathcal{E}$, and $[A]_{ij} = 0$ otherwise. Particularly, if the graph is undirected, then $A = A^\top$ and all its eigenvalues are real. When the digraph is simple, all the diagonal entries of A are zero. In what follows, we use $\lambda_1, \ldots, \lambda_n$ to denote the eigenvalues of A. The eigenvalue spectrum of A is denoted by $\texttt{spec}(A) = \{\lambda_i\}_{i=1}^n$. Moreover, the real part (respectively, imaginary part) of λ_i is denoted by σ_i (respectively, ω_i). Without loss of generality, we assume $|\lambda_1| \leq \cdots \leq |\lambda_n|$. The *spectral radius* of A is defined as $|\lambda_n|$. Furthermore, we denote $\omega_{\max}(A) = \max_i |\omega_i|$.

Two directed subgraphs, $G_s, G_h \subseteq G$, are said to be *isomorphic* [45], denoted by $G_s \simeq G_h$, if there exists a bijection $f : \mathcal{V}_s \to \mathcal{V}_h$ such that $(u,v) \in \mathcal{E}_s$ if and only if $(f(u), f(v)) \in \mathcal{E}_h$ for all $u, v \in \mathcal{V}_s$. When G_s and G_h are nonisomorphic, we write $G_s \not\simeq G_h$. In particular, when $\mathcal{V}_s = \mathcal{V}_h$, the bijection f is called an *automorphism* and the two directed subgraphs G_s and G_h are said to be *automorphic*, denoted by $G_s \overset{a}{\simeq} G_h$. Consequently, the $\simeq$ relation is an equivalence relation on the set of directed subgraphs of the same order, i.e., it classifies all possible directed subgraphs into equivalent classes. Based on these notions, we define the *isomorphic group* (respectively, *automorphic group*) of a directed subgraph $G_s \subseteq G$ by $\texttt{Iso}(G_s, G) = \{G_h \subseteq G : G_h \simeq G_s\}$ (respectively, $\texttt{Auto}(G_s, G) = \{G_h \subseteq G : G_h \overset{a}{\simeq} G_s\}$). Given a directed subgraph $G_s \subseteq G$, the *count* of G_s is defined by

$$\texttt{Count}(G_s, G) = \frac{|\texttt{Iso}(G_s, G)|}{|\texttt{Auto}(G_s, G)|}.$$

A digraph G is said to be *strongly connected* if there exists a path between every pair of vertices in G. A digraph G is said to be *weakly connected* if replacing all of its directed edges in $\mathcal{E}$ with undirected edges results in a connected (undirected) graph. Finally, let Ξ_s be the set of weakly connected digraphs of order s. We denote by $\Omega_s \subseteq \Xi_s$ the set of nonisomorphic strongly connected digraphs of order s.

3. Analysis of the spectral radius using subgraph counts.

In the following two subsections, we will establish a connection between the spectral moments of G and the counts of certain subgraphs. In subsection 3.3, we will exploit recent results regarding the existence of measures with a given sequence of moments to derive upper and lower bounds on the spectral radius of the graph in terms of these subgraph counts (presented in subsection 3.4). These bounds will be further refined in subsection 4.

3.1. From subgraphs to closed walks.

The eigenvalues of the adjacency matrix of a digraph are closely related to the walks within the digraph, as stated in the following lemma.

LEMMA 1 (see [46, section 6.5.2]). *Let A be the adjacency matrix of a simple digraph G. Given a positive integer k, $\mathrm{Tr}(A^k)$ is equal to the total number of closed walks of length k in G.*

Hereafter, we derive a relationship between the $\mathrm{Tr}(A^k)$ and the counts of subgraphs of different sizes. To illustrate the idea behind our approach with a simple case, let us decompose $\mathrm{Tr}(A^2)$ (i.e., $k = 2$) as follows:

$$\mathrm{Tr}(A^2) = \sum_{i=1}^{n}[A^2]_{ii} = \sum_{i=1}^{n}\sum_{j=1}^{n}[A]_{ij}[A]_{ji} = \sum_{i,j\colon (i,j),(j,i)\in\mathcal{E}} 1. \tag{3.1}$$

Note that the last term is counting (twice) the number of bidirected-edge subgraphs, i.e., pairs of vertices connected by two directed edges with reciprocal directions. For clarity, let us also consider the case $k = 3$. In this case, we can decompose the trace as

$$\mathrm{Tr}(A^3) = \sum_{i=1}^{n}[A^3]_{ii} = \sum_{i,j,k\colon (i,j),(j,k),(k,i)\in\mathcal{E}} 1. \tag{3.2}$$

Therefore, $\mathrm{Tr}(A^3)$ is equal to (three times) the number of directed triangles in G.

More generally, for given $k \in \mathbb{N}$, we prove the following theorem.

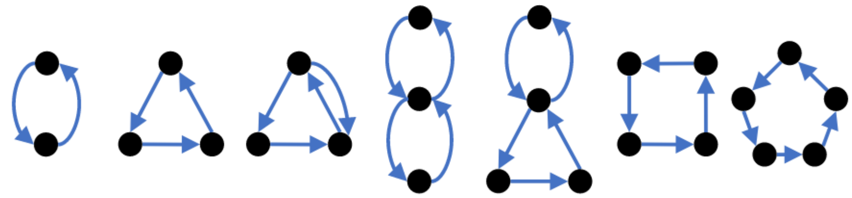
THEOREM 2. *Consider a (simple) digraph G with adjacency matrix A. For all $\widehat{G} \in \Omega_s$ and all positive integers k, we define $\eta(\widehat{G}, k)$ as the number of closed walks of length k in $\widehat{G}$ visiting all the edges of $\widehat{G}$ at least once. Then the following holds:*

$$\mathrm{Tr}(A^k) = \sum_{s=2}^{k}\sum_{\widehat{G}\in\Omega_s} \eta(\widehat{G}, k)\,\mathtt{Count}(\widehat{G}, G). \tag{3.3}$$

Proof. See Appendix A. ∎

Based on Theorem 2, we can fill a table with the values of $\eta(\widehat{G}, k)$ for different values of k (see Figure 3.1). The rows in this table are indexed by those subgraphs involved in the computation of the traces up to the fifth power. The coefficients in this table can then be used to compute $\mathrm{Tr}(A^k)$ for $k \leq 5$, as a linear combination of the counts of the subgraphs plotted in the table. For example, from the first row of the table, we infer that $\mathrm{Tr}(A^2)$ is equal to two times the count of bidirected-edge subgraphs. In other words, we have that $\eta(\widehat{G}, 2) = 2$, where $\widehat{G} \in \Omega_2$ is the bidirected-edge subgraph. Similarly, from the second row, we infer that $\mathrm{Tr}(A^3)$ equals three times the count of directed triangles. That is, $\mathrm{Tr}(A^3) = 3 \times \mathtt{Count}(\widehat{G}, G)$, in which $\eta(\widehat{G}, 3) = 3$ and $\widehat{G} \in \Omega_3$ is the directed triangle subgraph.

3.2. From subgraph counts to spectral moments. In this subsection, we derive a relationship between closed walks in G and the power sums of the eigenvalues in A. To achieve this goal, we first introduce some notions from probability theory. Let μ be a measure on $\mathbb{R}^n$. The support of μ, denoted by $\mathrm{Supp}(\mu)$, is defined as the smallest closed set $C \subseteq \mathbb{R}^n$ such that $\mu(\mathbb{R}^n \setminus C) = 0$ [47]. The measure μ is called r-atomic if $|\mathrm{Supp}(\mu)| = r$, i.e., a discrete set of cardinality r. The kth moment of an $\mathbb{R}$-valued random variable x is defined as $\mathbb{E}[x^k] = \int_{\mathbb{R}} x^k d\mu_x$, where μ_x is the corresponding probability measure of x. Given an $\mathbb{R}^n$-valued random variable $\mathbf{x}$ and an n-dimensional vector of integers $\boldsymbol{\alpha} \in \mathbb{N}^n$, we let $\mathbf{x}^{\boldsymbol{\alpha}} = \prod_{i=1}^{n} x_i^{\boldsymbol{\alpha}_i}$. Subsequently,



$\mathrm{Tr}(A^2)$	2	0	0	0	0	0	0
$\mathrm{Tr}(A^3)$	0	3	0	0	0	0	0
$\mathrm{Tr}(A^4)$	2	0	0	4	0	4	0
$\mathrm{Tr}(A^5)$	0	0	5	0	5	0	5

FIG. 3.1. *This table shows the values of $\eta(\widehat{G}, k)$, defined in Theorem 2, for $k \leq 5$. The value k indexes the powers of A in the rows (e.g., $k = 2$ in the first row and $k = 3$ in the second row). The columns of the table are indexed by all nonisomorphic strongly connected subgraphs of order at most 5 involved in the computation of the traces up to the fifth power (i.e., $k \leq 5$). For instance, from the second row of the table, where $k = 3$, we infer that $\mathrm{Tr}(A^3)$ equals 3 times the number of directed triangles (second column in the table).*

the $\boldsymbol{\alpha}$-moment of $\mathbf{x}$ is defined as $\mathbb{E}[\mathbf{x}^{\boldsymbol{\alpha}}] = \int_{\mathbb{R}^n} \prod_{i=1}^n x_i^{\boldsymbol{\alpha}_i} d\boldsymbol{\mu}$, where $\boldsymbol{\mu}$ is the probability measure of $\mathbf{x} = [x_1, \ldots, x_n]^\top$. Moreover, the *order* of $\boldsymbol{\alpha}$ is defined by $|\boldsymbol{\alpha}| = \sum_{i=1}^n \alpha_i$.

Given a digraph G, we define the *spectral measure* of its adjacency matrix A as the following two-dimensional probability density:

$$\mu_A(x, y) = \frac{1}{n} \sum_{i=1}^n \delta(x - \sigma_i)\delta(y - \omega_i), \tag{3.4}$$

where $\delta(\cdot)$ is the Dirac delta measure, i.e., the probability measure on $\mathbb{R}$ that assigns unit mass to the origin, and zero elsewhere. In other words, the spectral measure μ_A is a discrete probability measure on $\mathbb{R}^2$ assigning a mass $1/n$ to each one of the n points in the set $\{(\sigma_i, \omega_i)\}_{i=1}^n$. Furthermore, we define the $\boldsymbol{\alpha}$-spectral moments of G, where $\boldsymbol{\alpha} = [a, b]^\top \in \mathbb{N}^2$, as the $\boldsymbol{\alpha}$-moment of the spectral measure μ_A, given by

$$m_{\boldsymbol{\alpha}}(A) = \int_{\mathbb{R}^2} x^a y^b d\mu_A(x, y). \tag{3.5}$$

We also write $m_{ab}(A)$ as an abbreviation of $m_{\boldsymbol{\alpha}}(A)$. As demonstrated in [40], the spectral moments of an undirected graph can be computed as a linear combination of the counts of certain nonisomorphic subgraphs. Hereafter, we derive a similar relationship between the spectral moments of a digraph G and the counts of certain (directed) subgraphs contained in G. To achieve this goal, we start by deriving a closed-form expression of the $\boldsymbol{\alpha}$-spectral moments, as stated in the following lemma.

LEMMA 3. *Given a directed graph G with adjacency matrix A, it holds that*

$$\mathrm{Tr}\left(A^k\right) = \sum_{s=0}^{\lfloor k/2 \rfloor} \binom{k}{2s} (-1)^s \, n \, m_{k-2s,2s}(A) \text{ for all } k \in \mathbb{N}. \tag{3.6}$$

Proof. From (3.4) and (3.5), the $\boldsymbol{\alpha}$-moment of the spectral measure for $\boldsymbol{\alpha} = [a, b]^\top$

equals

$$\begin{aligned} m_{ab}(A) &= \int_{\mathbb{R}}\int_{\mathbb{R}} x^a y^b \frac{1}{n}\sum_{i=1}^{n} \delta(x-\sigma_i)\,\delta(y-\omega_i)\,dxdy \\ &= \frac{1}{n}\sum_{i=1}^{n}\left[\int x^a \delta(x-\sigma_i)\,dx\right]\left[\int y^b \delta(y-\omega_i)\,dy\right] \\ &= \frac{1}{n}\sum_{i=1}^{n} \sigma_i^a \omega_i^b, \end{aligned}$$

where σ_i and ω_i are the real and imaginary parts of the ith eigenvalue of A, respectively. Since $\mathrm{Tr}(A^k)$ equals the sum of the kth powers of the eigenvalues of A, we have that

$$\begin{aligned} \mathrm{Tr}\left(A^k\right) &= \sum_{i=1}^{n} (\sigma_i + j\omega_i)^k = \sum_{i=1}^{n}\sum_{r=0}^{k}\binom{k}{r} j^r \omega_i^r \sigma_i^{k-r} \\ &= \sum_{i=1}^{n}\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,\omega_i^{2s}\sigma_i^{k-2s} \\ &\quad + j\sum_{i=1}^{n}\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s+1}(-1)^s\,\omega_i^{2s+1}\sigma_i^{k-2s+1} \\ &= \sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\sum_{i=1}^{n}\omega_i^{2s}\sigma_i^{k-2s} \\ &\quad + j\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s+1}(-1)^s\sum_{i=1}^{n}\omega_i^{2s+1}\sigma_i^{k-2s+1} \\ &= \sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\, n\, m_{2s,k-2s}(A). \end{aligned}$$

Notice that the imaginary term vanishes in the last equality, since $\mathrm{Tr}\left(A^k\right)$ is a purely real quantity. ∎

Combining Theorem 2 and (3.6), we have that

$$\sum_{s=2}^{k}\sum_{\widehat{G}\in\Omega_s}\eta(\widehat{G},k)\,\mathtt{Count}(\widehat{G},G) = \sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\, n\, m_{k-2s,2s}(A) \tag{3.7}$$

for all $k \in \mathbb{N}$. This expression allows us to directly relate the moments of the spectral measure of A to the counts of certain subgraphs in G.

3.3. *K*-moment problem. In many practical applications, such as the analysis of large-scale social networks, we do not have access to the whole topology of the graph G. Therefore, it is not possible to explicitly compute the eigenvalues of A. However, it may be possible to retrieve local structural information in the form of subgraph counts by crawling the network (see, for example, [26, 48, 49] and the references therein). Since in this situation it is not possible to exactly compute all the eigenvalues of A, it would be interesting to have tools allowing us to infer spectral information, such as bounds on eigenvalues, from the counts of small subgraphs in G. This is the main aim of this paper.

As we will show below, the counts of certain subgraphs can be used to constrain the moments of the spectral measure, which can then be used to find bounds on the spectral radius. In particular, from the counts of certain subgraphs of order less than or equal to k, we can write down an equality constraint for linear combinations of spectral moments using (3.7). However, it may be possible to find many different spectral measures (with different supports) satisfying the linear constraints in (3.7). In what follows, we will exploit recent results in the multidimensional moment problem [43] to compute outer and inner bounds on the set of all possible spectral supports. This result will directly provide us with upper and lower bounds on the spectral radius of A.

To explain our approach, we first need to introduce the K-moment problem [43] and related notions. A sequence $\mathbf{y} = \{y_{\boldsymbol{\alpha}}\}$ indexed by $\boldsymbol{\alpha} \in \mathbb{N}^n$ is called a *multisequence*. We will use multisequences to index the moments of $\mathbb{R}^n$-valued random variables. In particular, given a $\mathbb{R}^2$-valued random variable $\mathbf{x} \sim \mu$ and an index $\boldsymbol{\alpha} = [a,b]^\top \in \mathbb{N}^2$, we will use the notation $y_{\boldsymbol{\alpha}} = y_{ab}$ to denote the $\boldsymbol{\alpha}$-moment of μ, i.e., $y_{ab} = \mathbb{E}[\mathbf{x}^{[a,b]^\top}] = \int_{\mathbb{R}^2} x^a y^b d\mu(x,y)$.

DEFINITION 1. *Let K be a closed subset of $\mathbb{R}^n$. Let $\mathbf{y}_{n,\infty} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^n}$ be an infinite real multisequence. A measure μ on $\mathbb{R}^n$ is said to be a K-representing measure for $\mathbf{y}_{n,\infty}$ if*

$$y_{\boldsymbol{\alpha}} = \int_{\mathbb{R}^n} \mathbf{x}^{\boldsymbol{\alpha}} d\mu(\mathbf{x}) \text{ for all } \boldsymbol{\alpha} \in \mathbb{N}^n \tag{3.8}$$

and

$$\mathtt{Supp}(\mu) \subseteq K. \tag{3.9}$$

If $\mathbf{y}_{n,\infty}$ has a K-representing measure, we say that $\mathbf{y}_{n,\infty}$ is K-feasible. Similarly, a finite real multisequence $\mathbf{y}_{n,2r} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^n,|\boldsymbol{\alpha}|\le 2r}$ is said to be K-feasible if there exists a measure μ with $\mathtt{Supp}(\mu) \subseteq K$ such that (3.8) holds for all $\boldsymbol{\alpha} \in \mathbb{N}^n_{2r}$.

In this paper, we are interested in the case when K is characterized by polynomial inequalities, as stated below.

DEFINITION 2. *A set $K \subseteq \mathbb{R}^n$ is called a* semialgebraic *set if there exist m polynomials $g_i : \mathbb{R}^n \to \mathbb{R}$ such that*

$$K = \{\mathbf{x} \in \mathbb{R}^n \colon g_i(\mathbf{x}) \ge 0 \text{ for all } i \in [m]\}. \tag{3.10}$$

A necessary and sufficient condition to determine whether a finite multisequence is K-feasible, restricted to the case when K is both semialgebraic and compact, can be stated in terms of linear matrix inequalities involving *moment matrices* and *localizing matrices*, defined below.

DEFINITION 3 (see [43]). *Let $\mathbf{y}_{n,2r} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^n_{2r}}$ be a finite real multisequence. The* moment matrix *of $\mathbf{y}_{n,2r}$, denoted by $M_r(\mathbf{y}_{n,2r})$, is defined as the real matrix indexed by $\mathbb{N}^n_r$ and has the entries*

$$[M_r(\mathbf{y}_{n,2r})]_{\boldsymbol{\alpha},\boldsymbol{\beta}} = y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} \tag{3.11}$$

for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}^n_r$.

In this paper, we consider a particular order while indexing the entries of the moment matrix, as described below. Consider $\mathbf{x} = [x_1, \ldots, x_n]^\top$, and let

$$\mathcal{M} = \{1, x_1, \ldots, x_n, x_1^2, x_1x_2, \ldots, x_n^2, \ldots, x_1^r, x_1^{r-1}x_2, \ldots, x_n^r\}$$

be the set of monomials with degree up to r, written in degree-lexicographic order. The cardinality[1] of $\mathcal{M}$ is given by $\binom{n+r}{n}$. Given an $\mathbb{R}^n$-valued random variable $\mathbf{x}$, suppose that $\mathbf{y}_{n,2r} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^n_{2r}}$ is a moment sequence of $\mathbf{x}$, i.e., $y_{\boldsymbol{\alpha}} = \mathbb{E}[\mathbf{x}^{\boldsymbol{\alpha}}]$ for all $\boldsymbol{\alpha} \in \mathbb{N}^n_{2r}$. Then, according to Definition 3, the moment matrix of $\mathbf{y}_{n,2r}$ is expressed entrywise by (3.11). In this case, we have

$$[M_r(\mathbf{y}_{n,2r})]_{\boldsymbol{\alpha},\boldsymbol{\beta}} = y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} = \mathbb{E}[\mathbf{x}^{\boldsymbol{\alpha}}\mathbf{x}^{\boldsymbol{\beta}}]$$

for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}^n_r$. The right-hand side of the above equality can be viewed as taking the expectation of the product between the $\boldsymbol{\alpha}$th and the $\boldsymbol{\beta}$th monomial in $\mathcal{M}$. We use degree-lexicographic ordering to locate these moments inside the moment matrix. Consequently, the exponent of the monomials in $\mathcal{M}$ index the columns and rows in $M_r(\mathbf{y}_{n,2r})$, as shown in the example below.

Example 1. Let $n = 2$, $r = 1$, and $\mathbf{y}_{2,2} = \{y_{00}, y_{01}, y_{10}, y_{11}, y_{02}, y_{20}\}$. Suppose $\boldsymbol{\alpha} = [0, 1]^\top$ and $\boldsymbol{\beta} = [1, 0]^\top$; then $[M_1(\mathbf{y}_{2,2})]_{\boldsymbol{\alpha},\boldsymbol{\beta}} = y_{11}$. Moreover, according to Definition 3, the moment matrix of $\mathbf{y}_{2,2}$ is

$$\begin{aligned} M_1(\mathbf{y}_{2,2}) &= \begin{bmatrix} \mathbb{E}\left[\mathbf{x}^{[00]^\intercal}\mathbf{x}^{[00]^\intercal}\right] & \mathbb{E}\left[\mathbf{x}^{[00]^\intercal}\mathbf{x}^{[10]^\intercal}\right] & \mathbb{E}\left[\mathbf{x}^{[00]^\intercal}\mathbf{x}^{[01]^\intercal}\right] \\ \mathbb{E}\left[\mathbf{x}^{[10]^\intercal}\mathbf{x}^{[00]^\intercal}\right] & \mathbb{E}\left[\mathbf{x}^{[10]^\intercal}\mathbf{x}^{[10]^\intercal}\right] & \mathbb{E}\left[\mathbf{x}^{[10]^\intercal}\mathbf{x}^{[01]^\intercal}\right] \\ \mathbb{E}\left[\mathbf{x}^{[01]^\intercal}\mathbf{x}^{[00]^\intercal}\right] & \mathbb{E}\left[\mathbf{x}^{[01]^\intercal}\mathbf{x}^{[10]^\intercal}\right] & \mathbb{E}\left[\mathbf{x}^{[01]^\intercal}\mathbf{x}^{[01]^\intercal}\right] \end{bmatrix} \\ &= \begin{bmatrix} y_{00} & y_{10} & y_{01} \\ y_{10} & y_{20} & y_{11} \\ y_{01} & y_{11} & y_{02} \end{bmatrix}. \end{aligned}$$

The *localizing matrix* of a multisequence $\mathbf{y}_{n,2r}$ with respect to a polynomial $g : \mathbb{R}^n \to \mathbb{R}$ is defined as follows.

DEFINITION 4. *Consider a polynomial of degree v, $g(\mathbf{x}) = \sum_{\boldsymbol{\gamma}\in\mathbb{N}^n_v} u_{\boldsymbol{\gamma}}\mathbf{x}^{\boldsymbol{\gamma}}$, and a finite multisequence $\mathbf{y}_{n,2r} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^n_{2r}}$. The localizing matrix of $\mathbf{y}_{n,2r}$ with respect to g, denoted by $L_r(g, \mathbf{y}_{n,2r})$, is defined by the real matrix*[2]

$$[L_r(g, \mathbf{y}_{n,2r})]_{\boldsymbol{\alpha},\boldsymbol{\beta}} = \sum_{\boldsymbol{\gamma}\in\mathbb{N}^n_v} u_{\boldsymbol{\gamma}} y_{\boldsymbol{\gamma}+\boldsymbol{\alpha}+\boldsymbol{\beta}} \tag{3.12}$$

for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}^n_r$.

Example 2. Consider Example 1 with $n = 2$ and $r = 1$. Suppose that $g(\mathbf{x}) = a - x_1 + x_2^2$; then $\mathbf{u} = \{u_{00}, u_{10}, u_{02}\}$ with $u_{00} = a, u_{10} = -1, u_{02} = 1$. Subsequently, according to (3.12), $L_1(g, \mathbf{y}_{2,2})$ equals

$$L_1(g, \mathbf{y}_{2,2}) = \begin{bmatrix} ay_{00} - y_{10} + y_{02} & ay_{10} - y_{20} + y_{12} & ay_{01} - y_{11} + y_{03} \\ ay_{10} - y_{20} + y_{12} & ay_{20} - y_{30} + y_{02} & ay_{11} - y_{21} + y_{13} \\ ay_{01} - y_{11} + y_{03} & ay_{11} - y_{21} + y_{13} & ay_{02} - y_{12} + y_{04} \end{bmatrix}.$$

Hereafter, whenever clear from the context, we adopt the shorthand notation M_r to represent $M_r(\mathbf{y}_{n,2r})$, and $L_r(g)$ to represent $L_r(g, \mathbf{y}_{n,2r})$.

A necessary and sufficient condition for a finite multisequence $\mathbf{y} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}^n_r}$ being K-feasible is stated below.

[1] The cardinality of the set $\mathcal{M}$ can be derived by a star-and-bar argument in combinatorial mathematics; see, for example, [47].

[2] As described above, the elements of this matrix are ordered using degree-lexicographic ordering of $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$.

THEOREM 4 (see [43]). *Let $K \subseteq \mathbb{R}^n$ be a semialgebraic set defined by* (3.10) *and* $v = \max_j \lceil \frac{deg(g_j)}{2} \rceil$. *Given a finite multisequence* $\mathbf{y}_{n,2r} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathbb{N}^n_{2r}}$, *there exists a* $\mathtt{rank}(M_{r-v})$*-atomic K-representing measure for* $\mathbf{y}_{n,2r}$ *if and only if*

$$\begin{aligned} &M_r(\mathbf{y}_{n,2r}) \succeq 0, \text{ and } L_{r-v}(g_j, \mathbf{y}_{n,2r}) \succeq 0 \text{ for all } j \in [m], \\ &\mathtt{rank}(M_r(\mathbf{y}_{n,2r})) = \mathtt{rank}(M_{r-v}(\mathbf{y}_{n,2r})). \end{aligned} \tag{3.13}$$

In addition to this theorem, we present a corollary that is useful in the development of our framework.

COROLLARY 1. *Let $K \subseteq \mathbb{R}^n$ be a semialgebraic set defined as in* (3.10) *and* $v = \max_j \lceil \frac{deg(g_j)}{2} \rceil$. *Given a finite multisequence* $\mathbf{y}_{n,2r} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathbb{N}^n_{2r}}$, *if* $\mathbf{y}_{n,2r}$ *is K-feasible, then*

$$M_r(\mathbf{y}_{n,2r}) \succeq 0, \text{ and } L_{r-v}(g_j \mathbf{y}_{n,2r}) \succeq 0 \text{ for all } j \in [m]. \tag{3.14}$$

Based on Theorem 4, one can verify whether a given multisequence is K-feasible by verifying the positive semidefiniteness of finitely many matrices. In the next subsection, we make use of Theorem 4 to provide upper and lower bounds on spectral radius of a directed graph given counts of subgraphs contained in G up to order r.

3.4. Lower bounds using the *K*-moment problem. In this subsection, we aim to obtain upper and lower bounds for the spectral radius of A by leveraging the connection between subgraph counts and the spectral moments of G, as shown in (3.7). To obtain a lower bound on the spectral radius, we use the theory behind the K-moment problem to characterize all K-feasible multisequences, $\mathbf{y}_{2,d} = \{y_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathbb{N}^2_d}$, for particular choices of K and integer[3] d. Following this idea, we next present necessary conditions for the existence of a *spectral* measure supported on K.

As shown in (3.7), the moments of a (spectral) measure must obey linear constraints imposed by the counts of certain subgraphs in G. In other words, if a multisequence $\mathbf{y}_{2,d}$ is a feasible spectral moment sequence, then there exists a spectral measure μ_A such that $y_{\boldsymbol{\alpha}} = \mathbb{E}_{\mu_A}[\mathbf{x}^{\boldsymbol{\alpha}}]$ for all $\boldsymbol{\alpha} \in \mathbb{N}^2_d$ (see Definition 1). Furthermore, according to (3.6), the entries of the sequence $\mathbf{y}_{2,d}$ must satisfy the linear constraints

$$\sum_{s=2}^{k} \sum_{\widehat{G} \in \Omega_s} \eta(\widehat{G}, k)\, \mathtt{Count}(\widehat{G}, G) = n \sum_{s=0}^{\lfloor k/2 \rfloor} \binom{k}{2s} (-1)^s\, y_{k-2s,2s} \tag{3.15}$$

for $k \in [d]$, where the left-hand side is a function of the counts of certain subgraphs of order up to d.

In addition to the above linear constraint, we notice that $\{\lambda_i\}_{i=1}^n$ are the eigenvalues of an adjacency matrix and that the eigenvalue spectrum of A is symmetric with respect to the real axis in the complex plane. Therefore, the moments of a spectral measure must satisfy

$$y_{ab} = 0 \text{ for } b \text{ odd.} \tag{3.16}$$

Furthermore, when a and b are both even, we have that $m_{ab}(A) = \frac{1}{n} \sum_{i=1}^n \sigma_i^a \omega_i^b \geq 0$. Therefore, the moments of a spectral measure must also satisfy

$$y_{ab} \geq 0 \text{ for } a \text{ and } b \text{ even.} \tag{3.17}$$

[3]As will be shown in later sections, the integer d represents the maximum size of all subgraphs whose counts are used in our computation for upper or lower bounds on λ_n.

Let us define $r = \lfloor \frac{d}{2} \rfloor$. In order to ensure that $\mathbf{y}_{2,d}$ is a feasible spectral moment sequence, the moment matrix defined by

$$[M_r]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} \text{ for } \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_r^2 \tag{3.18}$$

must be positive semidefinite according to Corollary 1. Furthermore, since A is entrywise nonnegative, the spectral radius of A equals λ_n according to Perron–Frobenius theory [50]. This also implies that $\omega_i \leq \rho$ for all $i \in [n]$ and $\rho = \lambda_n$. Consequently, the support of the spectral measure of A is contained in the square

$$S = \{\mathbf{x} \in \mathbb{R}^2 \colon x_1 \in [-\rho, \rho], x_2 \in [-\rho, \rho]\}.$$

Let $\mathbf{x} = [x_1, x_2]^\top$ and define the polynomials $g_1(\mathbf{x}) = \rho - x_1$, $g_2(\mathbf{x}) = x_1 + \rho$, $g_3(\mathbf{x}) = \rho - x_2$, and $g_4(\mathbf{x}) = x_2 + \rho$. The set S can be defined by

$$S = \{\mathbf{x} \in \mathbb{R}^2 \colon g_i(\mathbf{x}) \geq 0 \text{ for } i \in [4]\},$$

which is both compact and semialgebraic. According to Corollary 1, the localizing matrices of $\mathbf{y}_{2,d}$ with respect to $\{g_i\}_{i \in [4]}$ must be positive semidefinite. These matrices are given, entrywise, by

$$[L_r(g_1)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[1,0]^\top}, \tag{3.19}$$

$$[L_r(g_2)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} + y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[1,0]^\top}, \tag{3.20}$$

$$[L_r(g_3)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top}, \tag{3.21}$$

$$[L_r(g_4)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} + y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top} \tag{3.22}$$

for $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_r^2$. Therefore, the moment sequence $\mathbf{y}_{2,d}$ of the spectral measure of a matrix with spectral radius ρ must satisfy (3.15)–(3.17), and the moment and localizing matrices defined in (3.18)–(3.22) must be positive semidefinite.

Remark 1. Notice that, since $|\lambda_i| \leq \rho$ for all $i \in [n]$, the support of the spectral measure is also contained in the circle

$$S_c = \{[x, y]^\top \in \mathbb{R}^2 \colon x^2 + y^2 \leq \rho^2\}.$$

Defining $g_c = \rho^2 - x^2 - y^2$, we have that $S_c = \{[x, y]^\top \in \mathbb{R}^2 \colon g_c([x, y]^\top) \geq 0\}$. Therefore, the localizing matrix with respect to g_c of the moment sequence $\mathbf{y}_{2,d}$, given by

$$[L_r(g_c)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho^2 y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[2,0]^\top} - y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,2]^\top}, \tag{3.23}$$

must satisfy $L_{r-1}(g_c) \succeq 0$ for $\mathbf{y}_{2,d}$ to be a valid moment sequence of the spectral measure of a matrix with spectral radius ρ (see Corollary 1).

In what follows, we propose to find a lower bound on the spectral radius of A by solving a semidefinite program aiming to minimize the value of the parameter ρ in (3.19)–(3.23) while satisfying all the constraints described above. Subsequently, the solution to this semidefinite program renders a lower bound on the spectral radius of A, denoted by λ_n, as shown in the following theorem.

THEOREM 5. *Let r be an arbitrary positive integer and $d = 2r + 1$. Denote by $\underline{\rho}_r^\star$ the solution of the following semidefinite program:*

$$\begin{aligned} &\underset{\rho, \mathbf{y}_{2,d}}{\text{minimize}}\ \rho \\ &\textit{subject to}\ \ (3.15)\text{–}(3.17), \\ &\qquad\qquad\quad M_r \succeq 0, \\ &\qquad\qquad\quad L_r(g_i) \succeq 0 \textit{ for all } i \in [4], \end{aligned} \tag{3.24}$$

where M_r and $L_r(g_i)$ are defined in (3.18)–(3.22). Then $\underline{\rho}_r^\star \leq \lambda_n$ for all $r \in \mathbb{N}$. Furthermore, $\underline{\rho}_r^\star$ is a nondecreasing function of $r \in \mathbb{N}$.

Proof. See Appendix A. ∎

Remark 2. Since the support of the spectral measure is contained in *both* S and S_c, we can add constraint (3.23) in Remark 1 in conjunction with the constraints in (3.24). However, for a fixed value d, using (3.19)–(3.22) allows us to constraint more optimization variables in the optimization problem (3.24), hence giving us tighter bounds in practice. For instance, when $d = 5$ (i.e., $r = 2$), enforcing the spectral measure to be contained in S induces the following set of constraints: $L_2(g_i) \succeq 0$ for $i \in [4]$. This set of constraints poses constraints on optimization variables $y_{ab} \in \mathbf{y}_{2,5}$ with $a + b \leq 5$. On the contrary, if, as an alternative, (3.23) is applied, then we must have $L_1(g_c) \succeq 0$, which only provides constraint on variables of lower order, i.e., $y_{ab} \in \mathbf{y}_{2,5}$ with $a + b \leq 4$.

Theorem 5 allows us to compute a family of lower bound, parameterized by r, on the spectral radius of a digraph from counts of subgraphs up to order $d = 2r + 1$. In what follows, we provide a similar result to obtain a family of upper bounds on the spectral radius of A.

3.5. Upper bounds using the *K*-moment problem. From Perron–Frobenius theory [50], we know that the spectral radius of A is equal to the largest (nonnegative) real eigenvalue of A, denoted by λ_n. Hence, the set of eigenvalues $\lambda_1, \dots, \lambda_{n-1}$ must be contained inside a circle of radius λ_n, denoted by S_{λ_n}. In other words, if we define an auxiliary atomic density with $n - 1$ atoms located on the positions of the eigenvalues $\lambda_1, \dots, \lambda_{n-1}$, the multisequence of moments of this auxiliary density must be S_{λ_n}-feasible. Furthermore, we can consider a circle of radius ρ, denoted by S_ρ, and find the maximum value of ρ for which the multisequence of moments of the auxiliary density is S_ρ-feasible. This optimal value of ρ will provide us with an upper bound on the spectral radius λ_n. In what follows, we elaborate upon the details behind this approach.

We start our derivation with the following observation:

$$\sum_{s=2}^{k} \sum_{\widehat{G} \in \Omega_s} \eta(\widehat{G}, k)\, \texttt{Count}(\widehat{G}, G) = \lambda_n^k + \sum_{i=1}^{n-1} \lambda_i^k \tag{3.25}$$

for all $k \in \mathbb{N}$, which follows from (3.6). Let us introduce the following auxiliary atomic measure:

$$\tilde{\mu}_A(x, y) = \frac{1}{n-1} \sum_{i=1}^{n-1} \delta(x - \sigma_i)\delta(y - \omega_i). \tag{3.26}$$

We denote by $\tilde{m}_{\boldsymbol{\alpha}}$ the $\boldsymbol{\alpha}$-moment of $\tilde{\mu}_A$. In what follows, we use the theory behind the K-moment problem to derive necessary conditions that must be satisfied for all

K-feasible multisequences, $\mathbf{z}_{2,d} = \{z_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}\in\mathbb{N}_d^2}$, for particular choices of K. In our derivations, we make use of the following lemma.

LEMMA 6. *Given a directed graph G with adjacency matrix A, it holds that*

$$\mathrm{Tr}(A^k) = \lambda_n^k + (n-1)\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,\tilde{m}_{k-2s,2s} \text{ for all } k\in\mathbb{N}. \tag{3.27}$$

Proof. From (3.26), the $\boldsymbol{\alpha}$-moment of $\tilde{\mu}_A$ for $\boldsymbol{\alpha} = [a,b]^\top$ equals

$$\begin{aligned}\tilde{m}_{ab} &= \frac{1}{n-1}\int_{\mathbb{R}}\int_{\mathbb{R}} x^a y^b \sum_{i=1}^{n-1}\delta(x-\sigma_i)\,\delta(y-\omega_i)\,dxdy\\ &= \frac{1}{n-1}\sum_{i=1}^{n-1}\sigma_i^a\omega_i^b.\end{aligned} \tag{3.28}$$

From the proof of Lemma 3, we have that $m_{ab}(A) = \frac{1}{n}\sum_{i=1}^n \sigma_i^a\omega_i^b$. Combining this with (3.28), we have that

$$\tilde{m}_{ab} = \begin{cases}\dfrac{n}{n-1}m_{ab} & \text{if } b>0,\\ \dfrac{nm_{ab}-\sigma_n^a}{n-1} & \text{if } b=0.\end{cases} \tag{3.29}$$

Leveraging the connection between $m_{ab}(A)$ and $\mathrm{Tr}(A^k)$ (see (3.6)), we have

$$\begin{aligned}\mathrm{Tr}(A^k) &= n\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,m_{k-2s,2s}(A)\\ &= (n-1)\sum_{s=1}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,\tilde{m}_{k-2s,2s} + (n-1)\tilde{m}_{k,0} + \sigma_n^k\\ &= (n-1)\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,\tilde{m}_{k-2s,2s} + \sigma_n^k.\end{aligned}$$

Furthermore, according to Perron–Frobenius theory, we have that $\lambda_n = \sigma_n$. Thus, we obtain that

$$\mathrm{Tr}(A^k) = (n-1)\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,\tilde{m}_{k-2s,2s} + \lambda_n^k \tag{3.30}$$

for all $k\in\mathbb{N}$. ☐

If $\mathbf{z}_{2,d}$ is the moment multisequence for $\tilde{\mu}_A$, then $z_{\boldsymbol{\alpha}} = \mathbb{E}_{\tilde{\mu}_A}[\mathbf{x}^{\boldsymbol{\alpha}}]$ for all $\boldsymbol{\alpha}\in\mathbb{N}_d^2$ (see Definition 1). Furthermore, according to Lemma 6 and Theorem 2, the entries of the sequence $\mathbf{z}_{2,d}$ must satisfy the following linear constraint:

$$\sum_{s=2}^{k}\sum_{\widehat{G}\in\Omega_s}\eta(\widehat{G},k)\,\mathtt{Count}(\widehat{G},G) = (n-1)\sum_{s=0}^{\lfloor k/2 \rfloor}\binom{k}{2s}(-1)^s\,z_{k-2s,2s} + \rho^k \tag{3.31}$$

for $k \in [d]$. Moreover, similar to (3.16) and (3.17), we also have that

$$z_{ab} = 0 \text{ for } b \text{ odd,} \tag{3.32}$$

$$z_{ab} \geq 0 \text{ for } a \text{ and } b \text{ even.} \tag{3.33}$$

Notice that the support of $\tilde{\mu}_A(x, y)$ is contained in the square $S = [-\lambda_n, \lambda_n]^2$. Thus, the moment and localizing matrices corresponding to $\mathbf{z}_{2,d}$ have the same form as those in (3.18)–(3.22) after substituting $y_{\boldsymbol{\alpha}}$ by $z_{\boldsymbol{\alpha}}$. As a result, we obtain the following moment and localizing matrices:

$$[\tilde{M}_r]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = z_{\boldsymbol{\alpha}+\boldsymbol{\beta}}, \tag{3.34}$$

$$[\tilde{L}_r(g_1)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho z_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - z_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[1,0]^\top}, \tag{3.35}$$

$$[\tilde{L}_r(g_2)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho z_{\boldsymbol{\alpha}+\boldsymbol{\beta}} + z_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[1,0]^\top}, \tag{3.36}$$

$$[\tilde{L}_r(g_3)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho z_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - z_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top}, \tag{3.37}$$

$$[\tilde{L}_r(g_4)]_{\boldsymbol{\alpha}\boldsymbol{\beta}} = \rho z_{\boldsymbol{\alpha}+\boldsymbol{\beta}} + z_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top} \tag{3.38}$$

for $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{N}_r^2$. As required by Corollary 1, the moment matrix (3.34) and localizing matrices (3.35)–(3.38) must be positive semidefinite. As a result, for $\rho = \lambda_n$, the moment sequence $\mathbf{z}_{2,d}$ of the auxiliary spectral measure $\tilde{\mu}_A$ must satisfy (3.31)–(3.33) and the moment and localizing matrices in (3.34)–(3.38) must be positive semidefinite.

In what follows, we find an upper bound on the spectral radius by solving a semidefinite program whose objective is to maximize the value of the parameter ρ in (3.31)–(3.38), while satisfying all the aforementioned constraints, as described in the following theorem.

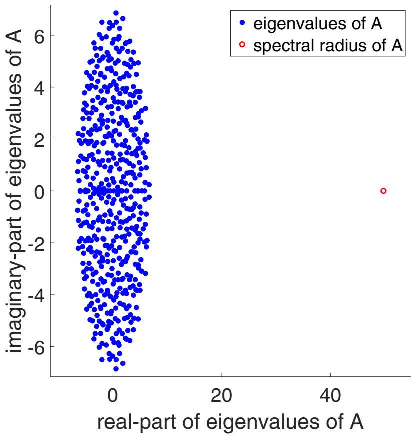
THEOREM 7. *Let r be an arbitrary positive integer and $d = 2r + 1$. Denote by $\overline{\rho}_r^\star$ the solution of the following semidefinite program:*

$$\begin{aligned} &\underset{\rho, \mathbf{z}_{2,d}}{\text{maximize}}\ \rho \\ &\textit{subject to } (3.31)\text{–}(3.33), \\ &\qquad\qquad \tilde{M}_r \succeq 0, \\ &\qquad\qquad \tilde{L}_r(g_i) \succeq 0 \textit{ for all } i \in [4], \end{aligned} \tag{3.39}$$

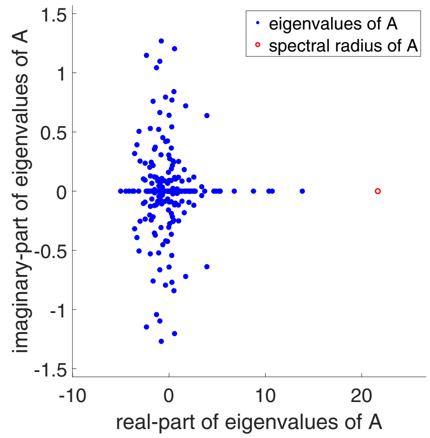
where $\tilde{M}_r$ and $\tilde{L}_r(g_i)$ are defined in (3.34)–(3.38). Then $\overline{\rho}_r^\star \geq \lambda_n$ for all $r \in \mathbb{N}$. Furthermore, $\overline{\rho}_r^\star$ is a nonincreasing function of $r \in \mathbb{N}$.

Using Theorems 5 and 7, we can compute lower and upper bounds on the spectral radius of a directed graph using counts of subgraphs in G. Furthermore, these bounds become tighter as the order of subgraphs under consideration increases.

3.6. Illustration and discussion. To demonstrate the performance of these bounds, we apply our methodology to a directed graph modeling the connections between $n = 1{,}574$ different airports within the United States [51]. Assuming we are able to count the number of all subgraphs of order up to 6, the upper bound



(a)



(b)

FIG. 3.2. *In* (a)*, we plot the complex eigenvalues of A for an Erdős–Rényi random directed graph with $n = 500$ vertices and edge probability* 0.1*. The spectral radius of A is $\lambda_n \approx 50$, whereas $\omega_{\max} < 7$. In* (b)*, we plot the complex eigenvalues of A for a real social network from Google+* [51]*. The spectral radius of $\lambda_n \approx 21$, whereas $\omega_{\max} < 1.5$.*

on the spectral radius obtained via Theorem 7 equals $\overline{\rho}_3^\star = 99.2906$, whereas the actual spectral radius equals $\lambda_n = 99.1183$. However, when we only have access to the counts of subgraphs of small order, our approach can lead to loose bounds. For example, considering a realization of the Erdős–Rényi random directed graph with $n = 100$ vertices and $\mathbb{P}((i,j) \in \mathcal{E}) = 0.15$ for all $i, j \in \mathcal{V}$, we obtain a spectral radius of $\lambda_n = 14.5431$. In this case, when the counts of subgraphs of order up to 4 are available, the lower bound obtained using Theorem 5 is $\underline{\rho}_2^\star = 5.5$. This bound is loose for the following two reasons: First, although Theorems 5 and 7 provide lower and upper bounds on the spectral radius, the moments of the optimal solutions may not correspond to an n-atomic measure, since Corollary 1 does not provide a sufficient condition to guarantee the existence of an n-atomic measure. Second, and more importantly, we have assumed that $\texttt{spec}(A)$ is contained in the square $[-\lambda_n, \lambda_n]^2$. However, the support of μ_A is contained in $[-\lambda_n, \lambda_n] \times [-\omega_{\max}, \omega_{\max}]$, where $\omega_{\max}$ can be much smaller than λ_n in some real digraphs, leading to loose bounds (see Figure 3.2). In the following section, we propose a refinement of our technique in order to overcome this issue by finding better bounds on ω_{max}.

4. Refined moment-based bounds.

In this section, we introduce a refined moment-based framework to improve the quality of our bounds on the spectral radius. The main idea behind this approach is to obtain an upper bound on $\omega_{\max}$. To achieve this goal, we will study the spectral measure of the matrix $A - A^\top$. As we discuss below, the largest imaginary part among the eigenvalues of $A - A^\top$ upper bounds ω_{max} of A. We then relate the spectral moments of $A - A^\top$ to the counts of certain subgraphs in G. Finally, we will resort to the K-moment problem to provide an upper bound on $\omega_{\max}$. This upper bound will be further used to provide refined upper and lower bounds on the spectral radius of A.

In order to provide an upper bound on $\omega_{\max}$ of A, we first present a connection between the eigenvalues of the (imaginary) matrix $A_I = j(A - A^\top)$ and those of A, where j is the imaginary unit that satisfies $j^2 = -1$. Notice that the matrix $A - A^\top$ is skew-symmetric; hence, its eigenvalues are a collection of purely imaginary conjugate pairs. Hence, the spectrum of A_I is purely real and symmetric around the imaginary axis. From [29], we have that

$$\omega_{\max} \leq \frac{1}{2} \max\{\mathbf{v}^* A_I \mathbf{v} : \mathbf{v}^*\mathbf{v} = 1, \mathbf{v} \in \mathbb{C}^n\} = \lambda_n(A_I),$$

where $\lambda_n(A_I)$ is the largest (real) eigenvalue of A_I. In particular, the equality holds if and only if A is normal. Using this relationship, we will provide an upper bound on $\omega_{\max}$ using traces of powers of A_I. In what follows, we show a linear relationship between counts of certain subgraphs in G and $\mathrm{Tr}(A_I^\ell)$.

4.1. From subgraph counts in G to traces of powers of A_I. Hereafter, we show that $\mathrm{Tr}(A_I^\ell)$ can be computed by a linear combination of the counts of specific subgraphs in G. To show this, we first provide a closed-form expression of the term $\mathrm{Tr}(A_I^\ell)$ using entries of A_I. On the one hand, since the spectrum of A_I is symmetric around the imaginary axis, we have that $\mathrm{Tr}(A_I^\ell) = 0$ for ℓ odd. On the other hand, when ℓ is an even number, we have that

$$\begin{aligned} \mathrm{Tr}(A_I^\ell) &= \mathrm{Tr}(j^\ell (A - A^\top)^\ell) \\ &= (-1)^{\frac{\ell}{2}} \mathrm{Tr}\left((A - A^\top)^\ell\right) \\ &= (-1)^{\frac{\ell}{2}} \sum_{\substack{c_i, d_i \in \{0,1\} \\ c_i + d_i = 1}} (-1)^{\sum_{i=1}^{\ell} d_i} \mathrm{Tr}\left[A^{c_1} (A^\top)^{d_1} \cdots A^{c_\ell} (A^\top)^{d_\ell}\right]. \end{aligned} \tag{4.1}$$

Therefore, $\mathrm{Tr}(A_I^\ell)$ is equal to the sum of 2^ℓ terms. Using ideas similar to those used in the proof of Theorem 2, one can show that $\mathrm{Tr}\left[A^{c_1} (A^\top)^{d_1} \cdots A^{c_\ell} (A^\top)^{d_\ell}\right]$ is equal to a linear combination of the counts of certain subgraphs in G. We illustrate this idea by considering the following examples.

Example 3. When $\ell = 2$, we have that

$$\begin{aligned} \mathrm{Tr}(A_I^2) &= -\mathrm{Tr}(A - A^\top)^2 \\ &= -\mathrm{Tr}(A^2 - AA^\top - A^\top A + (A^\top)^2) \\ &= -\mathrm{Tr}(A^2) + 2\mathrm{Tr}(AA^\top) - \mathrm{Tr}(A^\top)^2 \\ &= -2\mathrm{Tr}(A^2) + 2\mathrm{Tr}(AA^\top). \end{aligned} \tag{4.2}$$

In this particular case, we notice that $\mathrm{Tr}(A^2) = \sum_{i,j:(i,j),(j,i)\in\mathcal{E}} 1$ (see (3.1)) and $\mathrm{Tr}(AA^\top) = \sum_{i,j:(j,i)\in\mathcal{E}} 1$. The latter term equals the sum of in-degrees of each vertex i in G. Consequently, $\mathrm{Tr}(A_I^2)$ equals twice the total number of edges minus twice the counts of bidirected-edge subgraphs in G.

Let us consider an additional example when $\ell = 4$.

Example 4. When $\ell = 4$, we have that

$$\mathrm{Tr}(A_I^4) = \mathrm{Tr}((A - A^\top)^2 (A - A^\top)^2). \tag{4.3}$$

Using the properties of matrix trace operations, the above term is simplified to

$$\mathrm{Tr}(A_I^4) = 2\mathrm{Tr}(A^4) - 8\mathrm{Tr}(A^3 A^\top) + 4\mathrm{Tr}(A^2 (A^\top)^2) + 2\mathrm{Tr}((AA^\top)^2). \tag{4.4}$$

In what follows, we show that $\mathrm{Tr}(A^3 A^\top)$, $\mathrm{Tr}(A^2 (A^\top)^2)$, and $\mathrm{Tr}((AA^\top)^2)$ can all be calculated using the counts of certain subgraphs in G. We characterize those

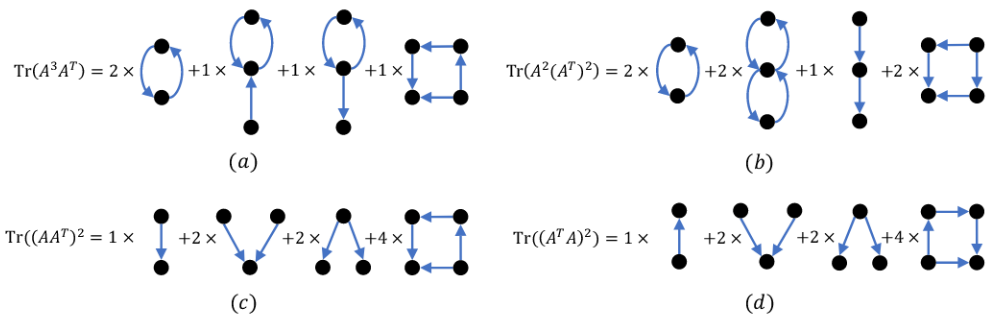


FIG. 4.1. *This figure shows the relationship between* $\mathrm{Tr}(A_I^4)$ *and the counts of certain subgraphs in* G. *More specifically, the traces in the figure are equal to sums of counts of certain subgraphs multiplied by the coefficients indicated in the figure. In* (c), *to calculate* $\mathrm{Tr}((AA^\top)^2)$, *we use the sum of in-degrees. In* (d), *to calculate* $\mathrm{Tr}((A^\top A)^2)$, *we use the sum of out-degrees. Since* $\mathrm{Tr}((AA^\top)^2) = \mathrm{Tr}((A^\top A)^2)$, *we can use either sum of in-degrees or sum of out-degrees to obtain* $\mathrm{Tr}((AA^\top)^2)$.

relationships in Figure 4.1. For demonstration purposes, we only show below the relationship between the term $\mathrm{Tr}((AA^\top)^2)$ and subgraph counts. Others traces can be computed in a similar fashion.

First, notice that

$$\mathrm{Tr}((AA^\top)^2) = \sum_i \sum_{j,k,l} [A]_{ij}[A]_{kj}[A]_{kl}[A]_{il}, \tag{4.5}$$

where the inside term is nonzero if and only if $(j,i),(j,k),(l,k),(l,i)$ are all edges of the digraph G. Next, we consider whether some of the indices $i,j,k,l \in [n]$ are equal. Since G is simple, $A_{ii} = 0$ for $i \in [n]$. Therefore, to ensure that $[A]_{ij}[A]_{kj}[A]_{kl}[A]_{il}$ is nonzero, it suffices to consider the following cases: (i) i,j,k,l are all distinct, (ii) $i = k$ while $j \neq l$, (iii) $i = k$ while $j = l$, and (iv) $i \neq k$ while $j = l$. In case (i), where i,j,k,l are all distinct, the ordered edges $(j,i),(j,k),(l,k),(l,i)$ together correspond to a subgraph of size four. However, notice that by permuting the indices, we obtain $(l,i),(l,k),(k,j),(j,i)$, which corresponds to the same subgraph (analogously for $(l,k),(l,i),(j,i),(j,k)$ and $(j,k),(j,i),(l,i),(l,k)$). As a result, the same subgraph is counted four times in the summation (4.5). Thus, the coefficient corresponding to this subgraph is 4 when calculating $\mathrm{Tr}((AA^\top)^2)$. In case (ii), the constraints given above induce a subgraph formed by the ordered sequence of edges $\{(j,i),(l,i)\}$, while $\{(l,i),(j,i)\}$ is another sequence representing the same subgraph. Thus, such a subgraph contributes twice in (4.5) and the associated coefficient is 2. In case (iii), $i = k$ and $j = l$, therefore $[A]_{ij}[A]_{kj}[A]_{kl}[A]_{il} = [A]_{ij}$, since A is unweighted. Hence, summing over all i in case (iii) corresponds to the sum of in-degrees of each vertex. Case (iv) is identical to case (ii).

Example 5. When $\ell = 6$, we have that

$$\begin{aligned}\mathrm{Tr}(A_I^6) = {} & 2\mathrm{Tr}(A^6) - 12\mathrm{Tr}(A^5A^\top) + 12\mathrm{Tr}(A^4(A^\top)^2)\\ & - 6\mathrm{Tr}(A^3(A^\top)^3) + 12\mathrm{Tr}(A^3A^\top AA^\top) + 6\mathrm{Tr}(A^2A^\top A^2A^\top)\\ & - 8\mathrm{Tr}(A^2(A^\top)^2AA^\top) - 4\mathrm{Tr}(A^2A^\top A(A^\top)^2) - 2\mathrm{Tr}(AA^\top AA^\top AA^\top).\end{aligned}$$

For all right-hand-side terms, we can apply analysis similar to that described in Example 4 to identify which subgraphs are present. More generally, for a particular sequence $\{(c_i,d_i)\colon c_i + d_i = 1, c_i, d_i \in \{0,1\}\}_{i=1}^{\ell}$, we can conclude a systematic

Algorithm 4.1. Identifying subgraphs whose counts are used to calculate $\mathrm{Tr}(A^{c_1}(A^\top)^{d_1}\cdots A^{c_\ell}(A^\top)^{d_\ell})$.

Input: Positive integer $\ell \in \mathbb{N}$.
Output: $\widetilde{G}_\ell$

Let $s = 0$ and $\widetilde{G}_s = \{\mathcal{V}_0, \mathcal{E}_0\}$, where $\mathcal{V}_0 = \{i_0\}$ and $\mathcal{E}_0 = \emptyset$.
for s $\leftarrow$ 1 to ℓ **do**
  if $c_s = 1$ **then**
    Let $\widetilde{G}_s = \{V_{s-1} \cup \{i_s\}, \mathcal{E}_{s-1} \cup \{(i_{s-1}, i_s)\}\}$, i.e., add an edge $i_{s-1} \to i_s$ to $\mathcal{E}_{s-1}$.
  else
    Let $\widetilde{G}_s = \{V_{s-1} \cup \{i_s\}, \mathcal{E}_{s-1} \cup \{(i_s, i_{s-1})\}\}$, i.e., add an edge $i_{s-1} \leftarrow i_s$ to $\mathcal{E}_{s-1}$.
  end if
end for
Let $i_\ell = i_0$ in $\widetilde{G}_\ell$.
Return $\widetilde{G}_\ell$.

procedure that is able to identify all subgraphs whose counts are used to calculate $\mathrm{Tr}(A^{c_1}(A^\top)^{d_1}\cdots A^{c_\ell}(A^\top)^{d_\ell})$. This procedure is summarized in Algorithm 4.1. From the output of Algorithm 4.1, the topology of each subgraph whose count is used to obtain $\mathrm{Tr}(A^{c_1}(A^\top)^{d_1}\cdots A^{c_\ell}(A^\top)^{d_\ell})$ can be constructed by considering a particular subset of vertices in $\widetilde{G}_\ell$ to be identical—see the four cases in Example 4 as an illustration. The coefficients of each of these subgraphs can be calculated using an idea similar to that introduced in Theorem 2.

Remark 3. Instead of $\mathrm{Tr}((AA^\top)^2)$, we may use $\mathrm{Tr}((A^\top A)^2)$ in (4.4) to obtain $\mathrm{Tr}(A_I^4)$. In this case, the subgraphs under consideration are listed in Figure 4.1(d). This observation can be generalized to all the terms involving traces of products of A and $A^\top$ in (4.1).

Remark 4. In general, finding a closed-form expression for the coefficients for the subgraphs using (4.1) is difficult. Moreover, to obtain $\mathrm{Tr}(A_I^r)$, one has to derive the counts for all subgraphs of size r, which can be computationally challenging when r is large. However, in most real networks, we obtain a tight approximation of the spectral radius by considering $r \leq 6$, as we will show empirically in section 5.

Next, we propose a method to upper bound the spectral radius of A_I using the K-moment problem.

4.2. Estimation of $\boldsymbol{\omega_{\max}(A)}$. To upper bound the spectral radius of A_I, we follow a procedure similar to the one discussed in the previous section. Given A_I, we define the spectral measure of A_I as the following one-dimensional probability density:

$$\nu_{A_I}(x) = \frac{1}{n}\sum_{i=1}^{n} \delta(x - \lambda_i(A_I)). \tag{4.6}$$

Since $\lambda_i(A_I) \in \mathbb{R}$, the measure ν_{A_I} is supported on $\mathbb{R}$. Without loss of generality, we can order the eigenvalues of A_I by $\lambda_1(A_I) \leq \cdots \leq \lambda_n(A_I)$. Since $A - A^\top$ is skew-symmetric, we have that $\lambda_1(A_I) = -\lambda_n(A_I)$. The support of ν_{A_I} must satisfy $\mathrm{Supp}(\nu(A_I)) \subseteq [-\lambda_n(A_I), \lambda_n(A_I)]$.

In addition to ν_{A_I}, we define the auxiliary spectral measure $\tilde{\nu}_{A_I}$ by

$$\tilde{\nu}_{A_I}(x) = \frac{1}{n-2} \sum_{i=2}^{n-1} \delta(x - \lambda_i(A_I)), \tag{4.7}$$

which is an $(n-2)$-atomic measure defined by removing both $\lambda_1(A_I)$ and $\lambda_n(A_I)$ from $\mathtt{spec}(A_I)$. Different from $\tilde{\mu}_A$, we remove two atoms from $\mathtt{spec}(A_I)$ to maintain the symmetry (with respect to the origin) of the auxiliary measure. Consequently, the supports of both ν_{A_I} and $\tilde{\nu}_{A_I}$ are contained in $[-\lambda_n(A_I), \lambda_n(A_I)]$.

Following an idea similar to the one presented in the previous section, we show that the trace of A_I^ℓ is related to the moments of both ν_{A_I} and $\tilde{\nu}_{A_I}$. More specifically, given a positive integer $r \in \mathbb{N}$, we compute the rth moment of ν_{A_I}, denoted by $m_r(A_I)$, as follows:

$$m_r(A_I) = \int_{x\in\mathbb{R}} x^r d\nu_{A_I} = \frac{1}{n} \sum_{i=1}^{n} \lambda_i(A_I)^r = \frac{1}{n}\mathrm{Tr}(A_I^r). \tag{4.8}$$

Similarly, the rth moment of $\tilde{\nu}_{A_I}$, denoted by $\tilde{m}_r(A_I)$, is equal to

$$\begin{aligned} \tilde{m}_r(A_I) &= \int_{x\in\mathbb{R}} x^r d\tilde{\nu}_{A_I} \\ &= \frac{1}{n-2} \sum_{j=2}^{n-1} \lambda_i(A_I)^r \\ &= \frac{1}{n-2} \left[\mathrm{Tr}(A_I^r) - ((-1)^r + 1)\, \lambda_n(A_I)^r\right] \\ &= \frac{1}{n-2} \left[n m_r(A_I) - ((-1)^r + 1)\, \lambda_n(A_I)^r\right]. \end{aligned} \tag{4.9}$$

To obtain an upper bound on $\lambda_n(A_I)$, we first find necessary conditions that must be satisfied by all moment sequences of $\tilde{\nu}_{A_I}$, denoted by $\mathbf{w}_{2r+1} = \{w_\gamma\}_{\gamma\le 2r+1}$. Since the spectrum of A_I is symmetric around 0, it follows that all odd moments of ν_{A_I} and $\tilde{\nu}_{A_I}$ are 0. As a result, in order for $\mathbf{w}_{2r+1}$ to be a moment sequence with respect to $\tilde{\nu}_{A_I}$, we must have

$$w_\gamma = \begin{cases} 1 & \text{if } \gamma = 1, \\ 0 & \text{if } \gamma > 1 \text{ and } \gamma \text{ is an odd number}, \\ \dfrac{1}{n-2}\left(\mathrm{Tr}(A_I^\gamma) - 2\lambda_n(A_I)^\gamma\right) & \text{otherwise} \end{cases} \tag{4.10}$$

for all $\gamma \le 2r+1$.

Moreover, the moment and localizing matrices of $\mathbf{w}_{2r+1}$ must be positive semidefinite, as required by Theorem 4. More specifically, we let the moment matrix of $\mathbf{w}_{2r+1}$ be defined entrywise by

$$[M_r(\mathbf{w})]_{\alpha,\beta} = w_{\alpha+\beta}, \tag{4.11}$$

where $\alpha, \beta \in \mathbb{N}_r$. Let $h_1(x) = x - \lambda_n(A_I)$ and $h_2(x) = x + \lambda_n(A_I)$; hence, we have that $[-\lambda_n(A_I), \lambda_n(A_I)] = \{x \in \mathbb{R} \colon h_1(x) \ge 0, h_2(x) \ge 0\}$. Next, we define the localizing matrices with respect to h_1 and h_2 by

$$[L_r(h_1, \mathbf{w})]_{\alpha,\beta} = \lambda_n(A_I) w_{\alpha+\beta} - w_{\alpha+\beta+1} \tag{4.12}$$

and

$$[L_r(h_2, \mathbf{w})]_{\alpha,\beta} = \lambda_n(A_I) w_{\alpha+\beta} + w_{\alpha+\beta+1}. \tag{4.13}$$

Since the support of $\tilde{\nu}_{A_I}$ is contained in $[-\lambda_n(A_I), \lambda_n(A_I)]$, both $L_r(h_1, \mathbf{w})$ and $L_r(h_, \mathbf{w})$ must be positive semidefinite.

Subsequently, for $\rho = \lambda_n(A_I)$, the moment sequence $\mathbf{w}_{2r+1} = \{w_\gamma\}_{\gamma \le 2r+1}$ of the auxiliary spectral measure $\tilde{\nu}_{A_I}$ must satisfy (4.10). Furthermore, the moment and localizing matrices defined in (4.11)–(4.13) must be positive semidefinite (by replacing $\lambda_n(A_I)$ with the parameter ρ). Next, we aim to find the maximum value of the parameter ρ such that all the constraints above are satisfied.

Theorem 8. *Let A be the adjacency matrix of a digraph G, and define $A_I = j(A - A^\top)$. Let r be an arbitrary positive integer. Denote by $\omega_r^\star$ the solution to the following semidefinite program:*

$$\begin{aligned} &\underset{\rho, \mathbf{w}_{2r+1}}{\text{maximize}}\ \rho \\ &\textit{subject to } (4.10), \\ &\qquad\qquad M_r(\mathbf{w}) \succeq 0, L_r(g_1, \mathbf{w}) \succeq 0, L_r(g_2, \mathbf{w}) \succeq 0, \end{aligned} \tag{4.14}$$

where $M_r(\mathbf{w})$ and $L_r(g_i, \mathbf{w})$ are defined in (4.11)–(4.13). *Then $\frac{\omega_r^\star}{2} \ge \omega_{\max}$ for all $r \in \mathbb{N}$. Furthermore, $\omega_r^\star$ is a nonincreasing function of $r \in \mathbb{N}$.*

Note that, as described in subsection 4.1, the values of $\mathrm{Tr}(A_I^\ell)$ in (4.10) can be computed using counts of subgraphs of G. Hence, we have that $w_r^\star$ can be obtained using counts of subgraphs solely, providing an upper bound on the maximum imaginary part in the spectrum of A.

Corollary 2. *Let A be the adjacency matrix of a digraph G. Given a positive integer $r \in \mathbb{N}$, let $w_r^\star$ be the optimal solution to* (4.14). *If $A = A^\top$, then $w_r^\star = 0$ for all positive integers $r \in \mathbb{N}$.*

Proof. When $A = A^\top$, $\mathrm{Tr}(A_I^\gamma) = 0$ for all $\gamma \in \mathbb{N}$. Therefore, from (4.21), given an even integer $\gamma \in \mathbb{N}$, we have that $(n-2)w_\gamma = -2\rho^\gamma$ (by replacing $\lambda_n(A_I)$ with the optimization parameter ρ). Since $M_r(\mathbf{w})$ is positive semidefinite, all its diagonal entries are nonnegative. As a consequence, ρ must equal to zero. Therefore, $w_r^\star = 0$. ∎

The above corollary shows that the upper bound on $\omega_{\max}(A)$ is tight when A is a symmetric matrix. Consequently, the refined framework can also be used to obtain tight bounds for undirected graphs.

4.3. Refined bounds on the spectral radius. In section 3, we have considered that the spectrum of A is contained in the square $S = [-\lambda_n, \lambda_n]^2$. However, more precisely, $\mathtt{spec}(A)$ is contained in a rectangle $\hat{S} = [-\lambda_n, \lambda_n] \times [-\omega_{\max}, \omega_{\max}]$. Consequently, we define the polynomials $\hat{g}_3(\mathbf{x}) = \omega_{\max} - x_2$ and $\hat{g}_4(\mathbf{x}) = \omega_{\max} + x_2$. As required by Corollary 1, the localizing matrices of $\mathbf{y}_{2,d}$ with respect to $\hat{g}_3$ and $\hat{g}_4$ must be positive semidefinite. In other words, we impose additional constraints on the feasible sets in the optimization problems (3.24) and (3.39). This procedure is summarized in Algorithm 4.2.

Consequently, we have utilized counts of different subgraphs to provide upper and lower bounds on the spectral radius. In general, $\omega_{\max}(A)$ is much smaller than $\rho(A)$. Thus, the obtained solution from Algorithm 4.2 achieves better performance than the approach in section 3. Notice that not all subgraphs are needed to compute $\mathrm{Tr}(A_I^\ell)$

Algorithm 4.2. Refined upper and lower bounds of λ_n.

Input: Positive integer $r \in \mathbb{N}$, and $\{\mathrm{Tr}(A_I^\ell), \mathrm{Tr}(A^\ell)\}_{l=1}^{2r+1}$
Output: Lower bound and upper bound on the spectral radius of G, denoted by $\underline{\varrho}_r^\star$ and $\overline{\varrho}_r^\star$, respectively.
1: Let $d = 2r + 1$.
2: Solve (4.14) and obtain $w_r^\star$.
3: Define matrices $L_r(\hat{g}_3)$ and $L_r(\hat{g}_4)$ entrywise by

$$[L_r(\hat{g}_3)]_{\boldsymbol{\alpha\beta}} = w_r^\star y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top} \text{ and}$$

$$[L_r(\hat{g}_4)]_{\boldsymbol{\alpha\beta}} = w_r^\star y_{\boldsymbol{\alpha}+\boldsymbol{\beta}} + y_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top}.$$

4: Define matrices $\widetilde{L}_r(\hat{g}_3)$ and $\widetilde{L}_r(\hat{g}_4)$ entrywise by

$$[\widetilde{L}_r(\hat{g}_3)]_{\boldsymbol{\alpha\beta}} = w_r^\star z_{\boldsymbol{\alpha}+\boldsymbol{\beta}} - z_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top} \text{ and}$$

$$[\widetilde{L}_r(\hat{g}_4)]_{\boldsymbol{\alpha\beta}} = w_r^\star z_{\boldsymbol{\alpha}+\boldsymbol{\beta}} + z_{\boldsymbol{\alpha}+\boldsymbol{\beta}+[0,1]^\top}.$$

5: Compute $\underline{\varrho}_r^\star$ via

$$\begin{aligned}
\underline{\varrho}_r^\star = \arg\min_{\rho,\mathbf{y}_{2,d}} & \rho \\
\text{subject to } & (3.15)\text{–}(3.17), \\
& M_r \succeq 0, \\
& L_r(g_i) \succeq 0 \text{ for } i \in [4] \\
& L_r(\hat{g}_3) \succeq 0, L_r(\hat{g}_4) \succeq 0.
\end{aligned} \tag{4.15}$$

6: Obtain $\overline{\varrho}_r^\star$ via

$$\begin{aligned}
\overline{\varrho}_r^\star = \arg\max_{\rho,\mathbf{z}_{2,d}} & \rho \\
\text{subject to } & (3.30)\text{–}(3.33), \\
& \widetilde{M}_r \succeq 0, \\
& \widetilde{L}_r(g_i) \succeq 0 \text{ for } i \in [4], \\
& \widetilde{L}_r(\hat{g}_3) \succeq 0, \widetilde{L}_r(\hat{g}_4) \succeq 0.
\end{aligned} \tag{4.16}$$

and $\mathrm{Tr}(A^\ell)$. For example, when we consider using subgraphs of order less than or equal to 5, we only need the counts of those subgraphs depicted in Figure 4.2.

Remark 5. The optimization programs in Algorithm 4.2 as well as (4.14) are solved using a standard computation package in convex optimizations [52]. Notice that the semidefinite programs considered in our framework are not dependent on the size of the digraph G, and thus they can be solved efficiently. As an example, consider $r = 3$ (i.e., $d = 7$); the matrices in (4.15) and (4.16) are in $\mathbb{R}^{7\times 7}$. In fact, the bottleneck in terms of computation comes from retrieving the counts of high-order subgraphs in G. A MATLAB implementation of Algorithm 4.2 can be found in [53].

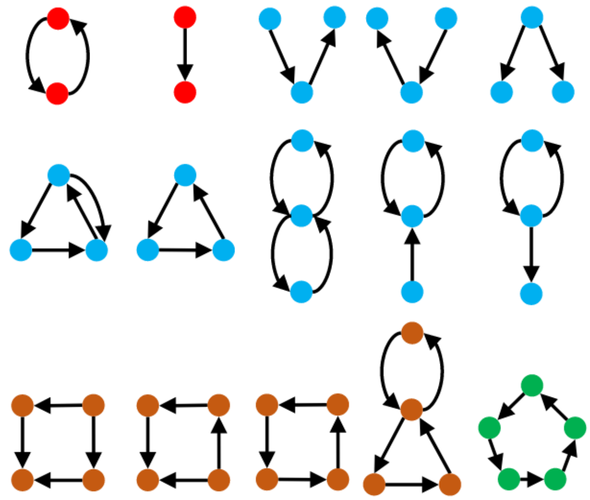


FIG. 4.2. *This figure shows those subgraphs whose counts are needed for estimating the spectral radius of A using Algorithm 4.2 with $r = 2$ (i.e., $d = 5$).*

4.4. Upper bound on $\boldsymbol{\lambda_n}$. We have proposed a framework to provide a more accurate estimate on the spectral radius of A using the relation between the imaginary parts of $\texttt{spec}(A)$ and $\texttt{spec}(A - A^\top)$. Similarly, we can also consider how the eigenvalues of $A_R = A + A^\top$ are related to the eigenvalues of A. More specifically, the relationship

$$\lambda_n \leq \frac{1}{2} \max\{\mathbf{v}^* A_R \mathbf{v} \colon \mathbf{v}^*\mathbf{v} = 1, \mathbf{v} \in \mathbb{C}^n\} = \frac{1}{2}\lambda_n(A_R), \tag{4.17}$$

where $\lambda_n(A_R)$ is the largest eigenvalue of A_R. In particular, the equality holds if and only if A is a normal matrix. As shown previously, an upper bound on $\lambda_n(A_R)$ can be obtained by relating the counts of a subsets of subgraphs in A to the spectral moments of $A + A^\top$. Therefore, this bound is also an upper bound for λ_n due to (4.17). Subsequently, we can also provide an upper bound on λ_n by providing an upper bound on $\lambda_n(A_R)$ using counts of subgraphs in G.

To characterize the upper bound on the spectral radius of A_R, we follow the idea presented in the previous subsection. Given A_R, we define the spectral measure of A_R as the following one-dimensional probability density:

$$\nu_{A_R}(x) = \frac{1}{n}\sum_{i=1}^{n} \delta(x - \lambda_i(A_R)). \tag{4.18}$$

We also define the $(n-1)$-atomic auxiliary spectral measure $\widetilde{\nu}_{A_R}$ by

$$\widetilde{\nu}_{A_R}(x) = \frac{1}{n-1}\sum_{i=1}^{n-1} \delta(x - \lambda_i(A_R)). \tag{4.19}$$

From the definitions of ν_{A_R} and $\widetilde{\nu}_{A_R}$, we compute the rth moment of $\widetilde{\nu}_{A_R}$, denoted by $\tilde{m}_r(A_R)$, as follows:

$$\begin{aligned}\tilde{m}_r(A_R) &= \int_{x\in\mathbb{R}} x^r d\tilde{\nu}_{A_R},\\ &= \frac{1}{n-1}\left[\mathrm{Tr}(A_R^r) - \lambda_n(A_R)^r\right].\end{aligned} \tag{4.20}$$

As illustrated in (4.5), as well as Theorem 2, $\mathrm{Tr}(A_R^r)$ can be computed using counts of certain subgraphs in G. As a consequence, $\tilde{m}_r(A_R)$ can also be computed as a linear combination of the counts of certain subgraphs in G. To find an upper bound on $\lambda_n(A_R)$, we provide below the necessary conditions that must be satisfied by all moment sequences of $\tilde{\nu}_{A_R}$, denoted by $\mathbf{p}_{2r+1}$.

According to (4.20), in order for $\mathbf{p}_{2r+1}$ to be a potential moment sequence of the density $\tilde{\nu}_{A_R}$, we must have

$$p_\gamma = \frac{1}{n-1}\left[\mathrm{Tr}(A_R^\gamma) - \lambda_n(A_R)^\gamma\right] \tag{4.21}$$

for all $\gamma \le 2r+1$. Moreover, the moment matrix of $\mathbf{p}_{2r+1}$, defined entrywise by

$$[M_r(\mathbf{p})]_{\alpha,\beta} = p_{\alpha+\beta} \tag{4.22}$$

for $\alpha,\beta \in \mathbb{N}_r$, must be positive semidefinite. Since $A \in \{0,1\}^{n\times n}$, the matrix $A_R = A + A^\top$ is entrywise nonnegative. It further follows that the largest eigenvalue of A_R is nonnegative, according to Perron–Frobenius theory. Subsequently, we have that $\mathtt{spec}(A_R) \subseteq [-\lambda_n(A_R), \lambda_n(A_R)]$. Let us define the polynomials $\phi_1(x) = \lambda_n(A_R) - x$ and $\phi_2(x) = \lambda_n(A_R)+x$; hence, we have that $\mathtt{spec}(A_R) \subseteq \{x \in \mathbb{R} \colon \phi_1(x) \ge 0, \phi_2(x) \ge 0\}$. Next, we define the localizing matrices with respect to ϕ_1 and ϕ_2 as

$$[L_r(\phi_1,\mathbf{p})]_{\alpha,\beta} = \lambda_n(A_R)p_{\alpha+\beta} - p_{\alpha+\beta+1}, \tag{4.23}$$

$$[L_r(\phi_2,\mathbf{p})]_{\alpha,\beta} = \lambda_n(A_R)p_{\alpha+\beta} + p_{\alpha+\beta+1} \tag{4.24}$$

for $\alpha,\beta \in \mathbb{N}_r$. Then Corollary 1 indicates that $L_r(\phi_1,\mathbf{p})$ and $L_r(\phi_2,\mathbf{p})$ must be positive semidefinite for the sequence $\mathbf{p}_{2r+1}$ to be a potential moment sequence of the density $\tilde{\nu}_{A_R}$.

Consequently, for $\rho = \lambda_n(A_R)$, the moment sequence $\mathbf{p}_{2r+1}$ of the auxiliary measure $\tilde{\nu}_{A_R}$ must satisfy the above constraints. The upper bound on $\lambda_n(A_R)$ can thus be found by maximizing the parameter ρ subjected to the above constraints, as shown in the following theorem.

THEOREM 9. *Let A be the adjacency matrix of a digraph G, and define $A_R = A + A^\top$. Let r be an arbitrary positive integer and $d = 2r+1$. Denote by $p_r^\star$ the optimal solution to the following semidefinite program:*

$$\begin{aligned}&\underset{\rho,\mathbf{p}_d}{\text{maximize}}\ \rho\\ &\textit{subject to } (4.21),\\ &\qquad\qquad M_r(\mathbf{p}) \succeq 0,\\ &\qquad\qquad L_r(\phi_1,\mathbf{p}) \succeq 0, L_r(\phi_2,\mathbf{p}) \succeq 0,\end{aligned} \tag{4.25}$$

where $M_r(\mathbf{p})$, $L_r(\phi_1,\mathbf{p})$, and $L_r(\phi_2,\mathbf{p})$ are defined in (4.22)–(4.24). Then $\frac{p_r^\star}{2} \ge \lambda_n$ for all $r \in \mathbb{N}$. Furthermore, $p_r^\star$ is a nonincreasing function of $r \in \mathbb{N}$.

Since $\mathrm{Tr}(A_R^\ell)$ can be computed using counts of subgraphs of G, we have that $p_r^\star$ can be obtained via counts of subgraphs of G.

5. Empirical results. In this section, we empirically demonstrate the validity of our bounds on random digraphs (subsection 5.1) and on real networks (subsection 5.2).

5.1. Random directed graphs. We generate random directed graphs according to the directed version of the Chung–Lu model [54]. More specifically, given a positive integer n, we consider two sequences $w_{in} = [w_1^{in}, w_2^{in}, \dots, w_n^{in}]^\top$ and $w_{out} = [w_1^{out}, w_2^{out}, \dots, w_n^{out}]^\top$, representing the in-degrees and out-degrees of each vertex. Furthermore, we let $\sum_{i=1}^n w_i^{in} = \sum_{i=1}^n w_i^{out} = m$. Then, according to [54], the entries in A are given by

$$A_{ij} = \begin{cases} 1 & \text{w.p. } \frac{w_i^{in} w_j^{out}}{m}, \\ 0 & \text{otherwise.} \end{cases} \tag{5.1}$$

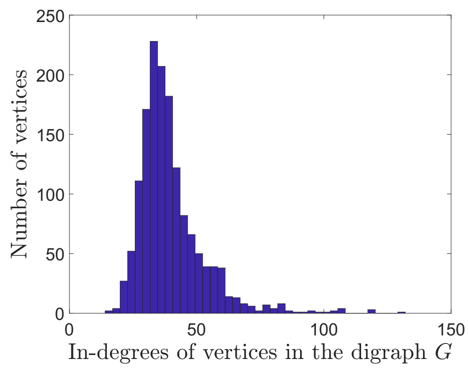
Using this model, we can also generate Erdős–Rényi random digraphs by letting $w_{in} = w_{out} = [pn, \dots, pn]^\top$ for a prescribed value $p \in (0, 1)$. As an example, we consider the following parameters in our experiment: $n = 500$ and $p = \frac{\log n}{n} \approx 0.0124$. Using these parameters, we generate a numerical realization of the random digraph A. The spectral radius of A equals $\lambda_n \approx 6.3002$, whereas $\omega_{\max} \approx 2.6373$. From Theorem 7, when $r = 2$, we have that $\rho_r^\star = 6.7806$.

In addition to Erdős–Rényi random digraphs, we can specify w_{in} and w_{out} to generate random graph power-law degree distributions. As shown in [55], given $c, \beta, i_0 \in \mathbb{R}$, we can define the sequence $w_i = c(i_0 + i)^{-\frac{1}{\beta-1}}$ to generate a random undirected graph whose degrees follow a power-law distribution with exponent β, i.e., the number of vertices with degree k is proportional to $k^{-\beta}$. In particular, it is possible to "control" the maximum degree, denoted by Δ, and average degree, denoted by d, by using the following parameter selection:

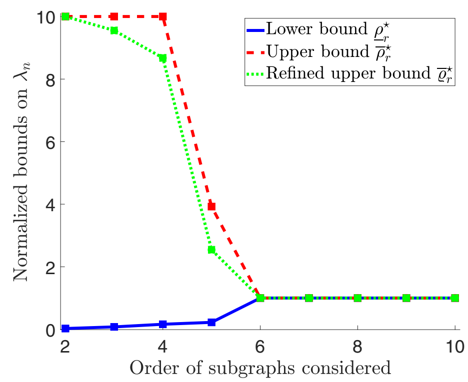
$$c = \frac{\beta - 2}{\beta - 1} d n^{\frac{1}{\beta-1}} \quad \text{and} \quad i_0 = n \left(\frac{d(\beta - 2)}{\Delta(\beta - 2)} \right)^{\beta - 1}. \tag{5.2}$$

In our experiment, we generate a sequence w using the above method and let $w_{in} = w_{out} = w$. In addition, we consider the following parameters: $n = 1500$, $\beta = 5$, $d = 40$, and $\Delta = 120$. Subsequently, from a random digraph realization, we have that $\lambda_n \approx 42.8770$, while $\omega_{\max} \approx 6.3868$. In Figure 5.1(a), we show the histogram of in-degrees for the particular random digraph realization under consideration, while in Figure 5.1(b), we show the evolution of the upper and lower bounds proposed in this paper as the order of the subgraph counts used increases. For example, the outputs of Algorithm 4.2 using counts of subgraphs of order up to 6 are an upper bound of 42.8777 and a lower bound of 42.8763, which are very tight in this case. Next, we explore our framework on real artificial directed graphs.

5.2. Real-world directed graphs. We consider several real digraphs obtained from [51] and [56]. In our first example, we examine the directed graph representing flights between U.S. airports in 2010 containing 1,574 vertices and 28,236 edges. In this digraph, each directed edge represents a flight connection from one airport to another. In our experiment, we preserve connectivity of the digraph and remove the edge weights. The spectral radius of the resulting (unweighted) digraph equals $\lambda_n = 99.1175$, whereas $\omega_{\max} = 2.881$. We plot the eigenvalue spectrum of A in Figure 5.2. Using the moment framework described in section 3, we obtain that our unrefined bounds are $\underline{\rho}_2^\star = 47.1184$ and $\overline{\rho}_2^\star = 172.2931$, when the counts of subgraphs of order up to 5 are considered. To improve these bounds, we first find an upper bound on



(a)



(b)

FIG. 5.1. *In* (a)*, we show the histogram of in-degrees of one realization of the Chung–Lu random digraph. In* (b)*, we show the normalized lower (solid line) and upper bounds, where the dashed and dotted lines show the upper bound obtained using Theorem* 5 *and Algorithm* 4.2*, respectively.*

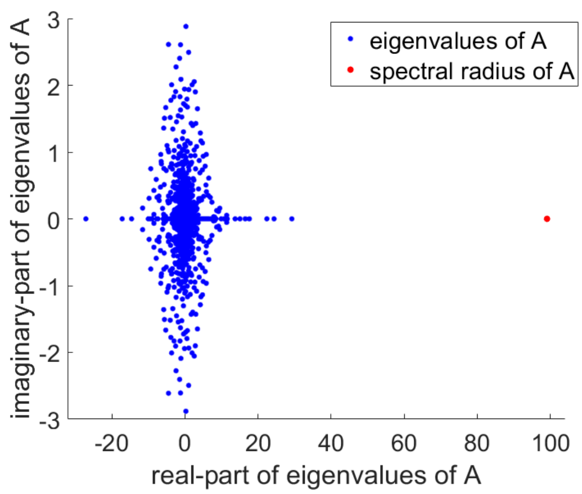


FIG. 5.2. *This figure shows the eigenvalue spectrum of the digraph representing flights between airports in the U.S. The x-axis and y-axis are the real and imaginary parts of the eigenvalues of A, respectively.*

$\omega_{\max}$. Using Algorithm 4.2, for $r = 2$, we obtained that $\omega_r^\star/2 \approx 8.2776$, which is an upper bound on $\omega_{\max}(A) = 2.881$. With the help on this additional information, we obtained that the refined lower bound and upper bound on the spectral radius equal 99.1167 and 102.9278, respectively.

In Tables 5.1 and 5.2, we illustrate the performance of our framework using other real-world directed graphs. In these experiments, we fix $r = 3$ and compare the performance of our bounds, with and without the refinement described in subsection 4.3. As previously indicated, the refined bounds are guaranteed to be no worse than the bounds obtained without estimating the largest imaginary part. Moreover, as r increases, the difference between the estimates using the two proposed methods

TABLE 5.1

This table shows lower bounds on the spectral radius of various networks computed using Theorem 5 (fifth column) and Algorithm 4.2 (last column).

Type	Size	λ_n	$\omega_{\max}$	$\underline{\rho}_3^\star$	$\underline{\varrho}_3^\star$
Social	131	18.3488	1.2132	8.0349	8.4347
Social	168	21.8484	0.8023	9.6100	13.5492
Social	344	21.6719	1.26	10.7704	21.6712
Social	627	10.4766	1.2995	5.2389	5.2389
Airport	1574	99.1175	2.881	99.1167	99.1167
Wikipedia	8297	47.9430	8.4824	29.9651	29.9651

TABLE 5.2

This table shows upper bounds computed using Theorem 7 (column 3, denoted by $\overline{\rho}_3^\star$), Theorem 9 (column 4, denoted by $p_3^\star$), and Algorithm 4.2 (last column), respectively.

Type	Size	λ_n	$\overline{\rho}_3^\star$	$p_3^\star$	$\overline{\varrho}_3^\star$
Social	131	18.3488	22.2728	22.5450	20.7786
Social	168	21.8484	35.9181	22.5630	24.9591
Social	344	21.6719	24.7768	29.6324	24.7768
Social	627	10.4766	12.8224	18.9572	12.3289
Airport	1574	99.1175	99.1183	99.2906	99.1183
Wikipedia	8297	47.9430	50.3321	49.0404	47.9438

diminishes, as illustrated in Tables 5.1 and 5.2. However, the convergence rate of our algorithm depends on the structure of the digraph. For example, we observe that, using $r = 3$, the lower bound returned by Algorithm 4.2 equals $\underline{\rho}_3^\star$ computed using Theorem 7 when we are considering the social network with $n = 627$ vertices.

6. Conclusion. The spectral radius of a digraph, i.e., the largest absolute value of its (complex) eigenvalues, is a graph metric that is relevant for the behavior of networked dynamical systems, such as epidemic processes, as well as graph-theoretic problems, such as the independence number or the graph diameter. In general, the spectral radius is a "global" graph metric, since its value cannot be computed unless the entire network topology is known. In this paper, we have shown that, given enough local information (i.e., subgraph counts), it is possible to approximate the spectral radius of large-scale networks. In particular, we have developed a novel mathematical framework to upper and lower bound the spectral radius of a digraph from the counts of a collection of small subgraphs. More specifically, by leveraging recent results on the K-moment problem, we have proposed a hierarchy of semidefinite programs of small size allowing us to compute sequences of upper and lower bounds on the spectral radius of a digraph using, solely, the counts of certain subgraphs. We have illustrated the quality of our bounds using both random digraphs and real-world directed networks.

Appendix A. Proofs of lemmas and theorems.

Proof of Theorem 2. Given $k \in \mathbb{N}$, we have

$$\begin{aligned}\operatorname{Tr}(A^k) &= \sum_{i=1}^{n} [A^k]_{ii},\\ &= \sum_{i=1}^{n} \sum_{j_1,\ldots,j_{k-1}} [A]_{ij_1} \cdots [A]_{j_{k-1}i}.\end{aligned} \tag{A.1}$$

In particular, since $[A]_{ii} = 0$ for all $i \in [n]$, we must have $i \neq j_1, j_{k-1} \neq i$ and $j_\ell \neq j_{\ell+1}$ for all $\ell < k-1$ in the above summation, since the term $[A]_{ij_1} \cdots [A]_{j_{k-1}i}$ vanished otherwise. We use $i \to j_1 \cdots j_{k-1} \to i$ to represent a closed walk of length k satisfying $[A]_{ij_1} \cdots [A]_{j_{k-1}i} \neq 0$. Notice that there may exist repetitive indices in $i \to j_1 \cdots j_{k-1} \to i$; hence, we may have that $|\{i, j_1, \ldots, j_{k-1}, i\}| \leq k$. Subsequently, we have

$$\sum_{j_1,\ldots,j_{k-1}} [A]_{ij_1} \cdots [A]_{j_{k-1}i} = \sum_{s=2}^{k} \sum_{|\{i,j_1,\ldots,j_{k-1},i\}|=s} [A]_{ij_1} \cdots [A]_{j_{k-1}i}. \tag{A.2}$$

In other words, we can classify closed walks into subgraphs with orders less than or equal to k. In particular, these subgraphs are weakly connected. Combining (A.2) and (A.1), we have

$$\operatorname{Tr}(A^k) = \sum_{i=1}^{n} \sum_{s=2}^{k} \sum_{|\{i,j_1,\ldots,j_{k-1},i\}|=s} [A]_{ij_1} \cdots [A]_{j_{k-1}i}. \tag{A.3}$$

Below, we analyze how the counts of order-k, weakly connected subgraphs contribute to (A.2).

Let us consider a subgraph $G_{sub} \subseteq G$ with order $s \leq k$. Without loss of generality, we may relabel the vertices of G_{sub} by $[s]$. Consider a closed walk of length k in G_{sub} such that the closed walk traverses each edge of G_{sub} at least once. Let $\eta_{i,k}(G_{sub})$ be the number of these closed walks starting at $i \in [n]$. Then each subgraph G_{sub} contributes $\sum_{i=1}^{s} \eta_{i,k}(G_{sub})$ number of walks in the summation in (A.3). Moreover, the number $\eta_{i,k}(G_{sub})$ is the same for all $G_h \in \texttt{Iso}(G_{sub})$. Let $\eta_k(G_{sub}) = \sum_{i=1}^{s} \eta_{i,k}(G_{sub})$. Then each class of subgraph contributes $\texttt{Count}(G_{sub}, G)\eta_k(G_{sub})$ to $\operatorname{Tr}(A^k)$. As a result,

$$\operatorname{Tr}(A^k) = \sum_{s=2}^{k} \sum_{G_{sub} \in \Omega_s} \texttt{Count}(G_{sub}, G)\eta_k(G_{sub}).$$

In particular, let A_s be the adjacency matrix of G_{sub}; if $\operatorname{Tr}[A_s^k] = 0$, then

$$\eta_{i,k}(G_{sub}) = 0$$

for all $i \in [s]$. ∎

Proof of Theorem 5. First, consider the spectral distribution μ_A and generate from μ_A an infinite multisequence $\mathbf{y}_{2,\infty}$ whose elements are given by $y_{\boldsymbol{\alpha}} = \mathbb{E}_{\mu_A}[\mathbf{x}^{\boldsymbol{\alpha}}]$ for all $\boldsymbol{\alpha} \in \mathbb{N}^2$. The discussions before Theorem 5 show that, given a fixed $r \in \mathbb{N}$, there exists a finite subsequence in $\mathbf{y}_{2,\infty}$ satisfying (3.15)–(3.17). Furthermore, according to Corollary 1, this subsequence satisfies $\tilde{M}_r \succeq 0, \tilde{L}_r(g_1) \succeq 0, \tilde{L}_r(g_2) \succeq 0, \tilde{L}_r(g_3) \succeq$

$0, \tilde{L}_r(g_4) \succeq 0$. In other words, all the constraints in (3.24) are satisfied. Thus, we can induce from $\mathbf{y}_{2,\infty}$ a *finite* subsequence of moments that is feasible with respect to (3.24). Consequently, the minimization in Theorem 5 leads to a lower bound on λ_n.

Similarly, for $r > 1$, we let $\mathcal{F}_r$ be the set of feasible solutions to (3.24). Since $\tilde{M}_r \succeq 0$, it follows that all its principal submatrices are positive semidefinite. Thus, $\tilde{M}_{r-1} \succeq 0$. Similar statements hold for $\tilde{L}_r(g_1), \tilde{L}_r(g_2), \tilde{L}_r(g_3)$, and $\tilde{L}_r(g_4)$. Thus, we have that $\mathcal{F}_r \subseteq \mathcal{F}_{r-1}$ and, consequently, $\rho^\star_{l,2r+1} \geq \rho^\star_{l,2r-1}$. ∎

Proof of Theorem 7. It suffices to replace μ_A in the proof of Theorem 5 by $\tilde{\mu}_A$. The rest of the proof of this theorem follows exactly the same logic as the proof of Theorem 5. ∎

Proof of Theorems 8 *and* 9. By replacing μ_A in the proof of Theorem 5 by $\tilde{\nu}_{A_I}$ and $\tilde{\nu}_{A_R}$, respectively, we can obtain that $p^\star_r \geq \lambda_n(A_R)$ and $\omega^\star_r \geq \lambda_n(A_I)$ for every $r \in \mathbb{N}$. Combining these bounds with

$$\omega_{\max}(A) \leq \lambda_n\left(\frac{j(A - A^\top)}{2}\right)$$

and

$$\lambda_n(A) \leq \lambda_n\left(\frac{A + A^\top}{2}\right),$$

the result follows. ∎

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