Structural Analysis of Laplacian Spectral Properties of Large-Scale Networks

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Abstract

Using methods from algebraic graph theory and convex optimization, we study the relationship between local structural features of a network and spectral properties of its Laplacian matrix. In particular, we derive expressions for the so-called spectral moments of the Laplacian matrix of a network in terms of a collection of local structural measurements. Furthermore, we propose a series of semidefinite programs to compute bounds on the spectral radius and the spectral gap of the Laplacian matrix from a truncated sequence of Laplacian spectral moments. Our analysis shows that the Laplacian spectral moments and spectral radius are strongly constrained by local structural features of the network. On the other hand, we illustrate how local structural features are usually not enough to estimate the Laplacian spectral gap.

I. Introduction

Understanding the relationship between the structure of a network and the behavior of dynamical processes taking place in it is a central question in the research field of network science [1]. Since the behavior of many networked dynamical processes is closely related with the Laplacian eigenvalues (see [2], [3] and references therein), it is of interest to study the relationship between structural features of the network and its Laplacian eigenvalues.

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In this technical note, we study this relationship, focusing on the role played by structural features that can be extracted from localized samples of the network structure. Our objective is then to efficiently aggregate these local samples of the network structure to infer global properties of the Laplacian spectrum. We propose a graph-theoretical approach to relate structural features of a network with algebraic properties of its Laplacian matrix. Our analysis reveals that there are certain spectral properties, such as the so-called spectral moments, that can be efficiently computed from these structural features. Furthermore, applying a recent result by Lasserre [4], we propose a series of semidefinite programs to compute bounds on the Laplacian spectral radius and spectral gap from a truncated sequence of spectral moments.

The paper is organized as follows. In the next subsection, we define terminology needed in our derivations. In Section II, we introduce a graph-theoretical methodology to derive closed-form expressions for the so-called Laplacian spectral moments in terms of structural features of the network. In Section III, we use semidefinite programming to derive optimal bounds on the Laplacian spectral radius and spectral gap from a truncated sequence of spectral moments. We validate our results numerically in Section IV.

A. *Notations & Preliminaries*

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be an undirected graph, where $\mathcal{V} = \{v_1, \ldots, v_n\}$ denotes a set of n nodes and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ denotes a set of e undirected edges. If $\{v_i, v_j\} \in \mathcal{E}$, we call nodes v_i and v_j *adjacent* (or first-neighbors), which we denote by $v_i \sim v_j$. We define the set of first-neighbors of a node v_i as $\mathcal{N}_i = \{w \in \mathcal{V} : \{v_i, w\} \in \mathcal{E}\}$. The *degree* d_i of a vertex v_i is the number of nodes adjacent to it, i.e., $d_i = |\mathcal{N}_i|$. We consider three types of undirected graphs: (*i*) A graph is called *simple* if its edges are unweighted and it has no self-loops[1], (*ii*) a graph is *loopy* if it has self-loops, and (*iii*) a graph is *weighted* if there is a real number associated with every edge in the graph. More formally, a weighted graph $\mathcal{H}$ can be defined as the triad $\mathcal{H} = (\mathcal{V}, \mathcal{E}, \mathcal{W})$, where $\mathcal{V}$ and $\mathcal{E}$ are the sets of nodes and edges in $\mathcal{H}$, and $\mathcal{W} = \{w_{ij} \in \mathbb{R}, \text{ for all } \{v_i, v_j\} \in \mathcal{E}\}$ is the set of (possibly negative) weights.

The *adjacency matrix* of a simple graph $\mathcal{G}$, denoted by $A_{\mathcal{G}} = [a_{ij}]$, is an $n \times n$ symmetric matrix defined entry-wise as $a_{ij} = 1$ if nodes v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. In

[1]A self-loop is an edge of the type $\{v_i, v_i\}$.

the case of weighted graphs (and possibly non-simple), the weighted adjacency matrix is defined by $W_{\mathcal{G}} = [w_{ij}]$, where $w_{ij} = 0$ if v_i is not adjacent to v_j. We define the *degree matrix* of a simple graph $\mathcal{G}$ as the diagonal matrix $D_{\mathcal{G}} = diag\,(d_i)$. We define the *Laplacian matrix* $L_{\mathcal{G}}$ (also known as combinatorial Laplacian, or Kirchhoff matrix) of a simple graph as $L_{\mathcal{G}} = D_{\mathcal{G}} - A_{\mathcal{G}}$. For simple graphs, $L_{\mathcal{G}}$ is a symmetric, positive semidefinite matrix, which we denote by $L_{\mathcal{G}} \succeq 0$ [5]. Thus, $L_{\mathcal{G}}$ has a full set of n real and orthogonal eigenvectors with real nonnegative eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n$. The second smallest and largest eigenvalues of $L_{\mathcal{G}}$, λ_2 and λ_n, are called the spectral gap and spectral radius of $L_{\mathcal{G}}$, respectively. Given a $n \times n$ real and symmetric matrix B with (real) eigenvalues $\sigma_1, ..., \sigma_n$, we define the k-th spectral moment of B as $m_k\,(B) \triangleq \frac{1}{n} \sum_{i=1}^{n} \sigma_i^k$. As we shall show in Section II, there is an interesting connection between the spectral moments of the Laplacian matrix, $m_k\,(L_{\mathcal{G}})$, and structural features of the network.

We now define a collection of structural properties that are important in our derivations. The *degree sequence* of a simple graph $\mathcal{G}$ is the ordered list of its degrees, $(d_1, ..., d_n)$. A *walk* of length k from v_{i_1} to $v_{i_{k+1}}$ is an ordered sequence of nodes $\left(v_{i_1}, v_{i_2}, ..., v_{i_{k+1}}\right)$ such that $v_{i_j} \sim v_{i_{j+1}}$ for $j = 1, 2, ..., k$. One says that the walk *touches* each of the nodes that comprises it. If $v_{i_1} = v_{i_{k+1}}$, then the walk is closed. A closed walk with no repeated nodes (with the exception of the first and last nodes) is called a *cycle*. Given a walk $p = \left(v_{i_1}, v_{i_2}, ..., v_{i_{k+1}}\right)$ in a weighted graph $\mathcal{H}$, we define the weight of the walk as, $\omega\,(p) = w_{i_1 i_2} w_{i_2 i_3} ... w_{i_k i_{k+1}}$.

II. Moment-Based Analysis of the Laplacian Matrix

In this paper, we use algebraic graph theory to study the relationship between structural properties of a network and its Laplacian spectrum based on the spectral moments. A well-known result in algebraic graph theory relates the diagonal entries of the k-th power of the adjacency matrix, $\left[A_{\mathcal{G}}^k\right]_{ii}$, to the number of closed walks of length k in G that start and finish at node v_i [5]. Using this result, it is possible to relate algebraic properties of the adjacency matrix $A_{\mathcal{G}}$ to the presence of certain subgraphs in the network [6]. We can generalize this result to weighted graphs as follows:

Proposition 1: Let $\mathcal{H} = (\mathcal{V}, \mathcal{E}, \mathcal{W})$ be a weighted graph with weighted adjacency matrix $W_{\mathcal{H}} = [w_{ij}]$. Then, $\left[W_{\mathcal{H}}^k\right]_{ii} = \sum_{p \in P_{k,i}} \omega\,(p)$,where $P_{k,i}$ is the set of closed walks of length k from v_i to itself in $\mathcal{H}$.

Proof: By recursively applying the multiplication rule for matrices, we have the following expansion

$$\left[W_{\mathcal{H}}^{k}\right]_{ii}=\sum_{i=1}^{n}\sum_{i_2=1}^{n}\cdots\sum_{i_k=1}^{n}w_{i,i_2}w_{i_2,i_3}\cdots\ w_{i_k,i}. \tag{1}$$

Using the graph-theoretic nomenclature introduced in Section I-A, we have that $w_{i,i_2}w_{i_2,i_3}...w_{i_k,i}=\omega\left(p\right)$, for $p=\left(v_i,v_{i_2},v_{i_3},...,v_{i_k},v_i\right)$. Hence, the summations in (1) can be written as $\left[W_{\mathcal{H}}^{k}\right]_{ii}=\sum_{1\leq i,i_2,...,i_k\leq n}\omega\left(p\right)$. Finally, the set of closed walks $p=\left(v_i,v_{i_2},v_{i_3},...,v_{i_k},v_i\right)$ with indices $1\leq i,i_2,...,i_k\leq n$ is equal to the set of closed walks of length k from v_i to itself in $\mathcal{H}$ (which we have denoted by $P_{k,i}$ in the statement of the Proposition). ■

The above Proposition allows us to write the relate moments of the weighted adjacency matrix of a weighted graph $\mathcal{H}$ to closed walks in $\mathcal{H}$, as follows:

Lemma 2.1: Let $\mathcal{H}=\left(\mathcal{V},\mathcal{E},\mathcal{W}\right)$ be a weighted graph with weighted adjacency matrix $W_{\mathcal{H}}=\left[w_{ij}\right]$. Then,

$$m_k\left(W_{\mathcal{H}}\right)=\frac{1}{n}\sum_{v_i\in\mathcal{V}}\sum_{p\in P_{k,i}}\omega\left(p\right),$$

where $P_{k,i}$ is the set of closed walks of length k from v_i to itself in $\mathcal{H}$.

Proof: Let us denote by $\mu_1,...,\mu_n$ the set of (real) eigenvalues of the (symmetric) weighted adjacency matrix $W_{\mathcal{H}}$. We have that the moments can be written as

$$m_k\left(W_{\mathcal{H}}\right)\triangleq\frac{1}{n}\sum_{i=1}^{n}\mu_i^k=\frac{1}{n}\text{Trace}\left(W_{\mathcal{H}}^{k}\right),$$

since $W_{\mathcal{H}}$ is a symmetric (and diagonalizable) matrix. We then apply Proposition 1 to rewrite the moments as follows,

$$m_k\left(W_{\mathcal{H}}\right)=\frac{1}{n}\sum_{i=1}^{n}\left[W_{\mathcal{H}}^{k}\right]_{ii}=\frac{1}{n}\sum_{v_i\in\mathcal{V}}\sum_{p\in P_{k,i}}\omega\left(p\right).$$

■

In Subsections II-B, we shall apply this result to compute spectral moments of the Laplacian matrix in terms of structural features of the network. First, we need to introduce a weighted graph that is useful in our derivations:

Definition 2.1: Given a simple graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, we define the Laplacian graph of $\mathcal{G}$ as the weighted graph $\mathcal{L}(\mathcal{G}) \triangleq (\mathcal{V}, \mathcal{E} \cup \mathcal{S}_n, \Gamma)$, where $\mathcal{S}_n = \{\{v, v\} \text{ for all } v \in \mathcal{V}\}$ (the set of all self-loops), and $\Gamma = [\gamma_{ij}]$ is a set of weights defined as:

$$\gamma_{ij} \triangleq \begin{cases} -1, & \text{for } \{v_i, v_j\} \in \mathcal{E} \\ d_i, & \text{for } i = j \\ 0, & \text{otherwise.} \end{cases}$$

Remark 2.1: Note that the weighted adjacency matrix of the Laplacian graph $\mathcal{L}(\mathcal{G})$ is equal to the Laplacian matrix of the simple graph $\mathcal{G}$. Hence, we can apply Lemma 2.1 to express the spectral moments of the Laplacian matrix $L_{\mathcal{G}}$ in terms of weighted walks in the Laplacian graph $\mathcal{L}(\mathcal{G})$.

Before we apply Lemma 2.1 to study the Laplacian spectral moments, we must introduce the concept of subgraph covered by a walk.

Definition 2.2: Consider a walk $p = \left(v_{i_1}, v_{i_2}, ..., v_{i_{k+1}}\right)$ of length k in a (possibly loopy) graph. We define the subgraph covered by p as the simple graph $C(p) = (\mathcal{V}_c(p), \mathcal{E}_c(p))$, with node-set $\mathcal{V}_c(p) = \bigcup_{r=1}^{k+1} v_{i_r}$, and edge-set $\mathcal{E}_c(p) = \bigcup_{v_{i_r} \neq v_{i_{r+1}}} \left\{v_{i_r}, v_{i_{r+1}}\right\}$, for $1 \leq r \leq k+1$.

Based on the above, we define *triangles*, *quadrangles* and *pentagons* as the subgraphs covered by cycles of length three, four, and five, respectively. Notice that self-loops are excluded from $\mathcal{E}_c(p)$ in Definition 2.2. For example, consider a walk $p = (v_1, v_2, v_2, v_3, v_3, v_1, v_3, v_1)$ in a graph with self-loops. Then, $C(p)$ has node-set $\mathcal{V}_c(p) = \{v_1, v_2, v_3\}$ and edge-set $\mathcal{E}_c(p) = \{\{v_1, v_2\}, \{v_2, v_3\}, \{v_3, v_1\}\}$. In other words, $C(p)$ is a simple triangle.

In what follows, we build on the above results to derive closed-form expressions for the first five spectral moments of the Laplacian matrix in terms of relevant structural features of the network.

A. Low-Order Laplacian Spectral Moments

The following theorem, proved in [7] via algebraic techniques, allows us to compute the first three Laplacian spectral moments in terms of the degree sequence and the number of triangles in the graph.

Theorem 2.2: Let $\mathcal{G}$ be a simple graph with Laplacian matrix $L_{\mathcal{G}}$. Then, the first three spectral moments of the Laplacian matrix are

$$
\begin{aligned}
m_1\left(L_{\mathcal{G}}\right) &= \frac{1}{n} S_1, \\
m_2\left(L_{\mathcal{G}}\right) &= \frac{1}{n}\left(S_1 + S_2\right), \\
m_3\left(L_{\mathcal{G}}\right) &= \frac{1}{n}\left(3S_2 + S_3 - 6\Delta\right),
\end{aligned}
\tag{2}
$$

where $S_p \triangleq \sum_{v_i \in \mathcal{V}} d_i^p$, and Δ is the total number of triangles in $\mathcal{G}$.

In [7], Theorem 2.2 was proved using a purely algebraic approach. This algebraic approach presents the limitation of not being applicable to compute moments of order greater than three. In what follows, we propose an alternative graph-theoretical approach that allows to compute higher-order spectral moments of the Laplacian matrix, beyond the third order. In particular, according to Lemma 2.1, we can compute the k-th spectral moment of the Laplacian of $\mathcal{G}$ by analyzing the set of closed walks of length k in the Laplacian graph $\mathcal{L}\left(\mathcal{G}\right)$.

B. *Higher-Order Laplacian Spectral Moments*

In this Subsection, we apply the set of graph-theoretical tools introduced above to compute the fourth- and fifth-order spectral moments of the Laplacian matrix. We first define the collection of structural measurements that are involved in our expressions. Let us denote by t_i, q_i, and p_i the number of triangles, quadrangles, and pentagons touching node v_i in $\mathcal{G}$, respectively. The total number of quadrangles and pentagons in $\mathcal{G}$ are denoted by Q and P, respectively. The following terms define structural correlations that are relevant in our analysis:

$$
\begin{aligned}
C_{dd} &\triangleq \frac{1}{n} \sum_{v_i \sim v_j} d_i d_j, \quad C_{d^2 d} \triangleq \frac{1}{n} \sum_{v_i \sim v_j} d_i^2 d_j, \\
C_{dt} &\triangleq \frac{1}{n} \sum_{v_i \in \mathcal{V}} d_i t_i, \quad C_{d^2 t} \triangleq \frac{1}{n} \sum_{v_i \in \mathcal{V}} d_i^2 t_i, \\
C_{dq} &\triangleq \frac{1}{n} \sum_{v_i \in \mathcal{V}} d_i q_i, \quad D_{dd} \triangleq \frac{1}{n} \sum_{v_i \sim v_j} d_i d_j \left|\mathcal{N}_i \cap \mathcal{N}_j\right|,
\end{aligned}
\tag{3}
$$

where $\left|\mathcal{N}_i \cap \mathcal{N}_j\right|$ is the number of common neighbors shared by v_i and v_j. The main result in this section relates the fourth and fifth Laplacian spectral moments to local structural measurements and correlation terms, as follows:

Theorem 2.3: Let $\mathcal{G}$ be a simple graph with Laplacian matrix $L_{\mathcal{G}}$. Then, the fourth and fifth Laplacian moments can be written as

$$\begin{aligned} m_4\left(L_{\mathcal{G}}\right) &= \frac{1}{n}\left(-S_1 + 2S_2 + 4S_3 + S_4 + 8Q\right) \\ &\quad +4C_{dd} - 8C_{dt}, \\ m_5\left(L_{\mathcal{G}}\right) &= \frac{1}{n}\left(-5S_2 + 5S_3 + 5S_4 + S_5 + 30\Delta - 10P\right) \\ &\quad +10\left(C_{dd} + C_{d^2d} - C_{dt} - C_{d^2t} + C_{dq} - D_{dd}\right) \end{aligned} \tag{4}$$

where $S_p \triangleq \sum_{v_i \in \mathcal{V}} d_i^p$, and the correlation terms C_{dd}, C_{dt}, C_{dq}, C_{d^2d}, C_{d^2t}, and D_{dd} are defined in (3).

Proof: In the Appendix. ■

Remark 2.2: Theorem 2.2 relates purely algebraic properties – the spectral moments – to structural features of the network, namely the degree sequence, the number of cycles of length 3 and 5, and all the correlation terms defined in (3). The key steps behind the proof are: (i) Relate the spectral moments $m_4\left(L_{\mathcal{G}}\right)$ and $m_5\left(L_{\mathcal{G}}\right)$ with closed walks of length four and five in the Laplacian graph $L\left(\mathcal{G}\right)$, and (ii) classify the set of closed walks in $L\left(\mathcal{G}\right)$ into subsets according to the subgraph covered by each walk.

In the next section, we present a series of semidefinite programs (SDP's) whose solutions provide optimal bounds on the Laplacian spectral radius and spectral gap in terms of Laplacian spectral moments.

III. Optimal Laplacian Bounds from Spectral Moments

In this section, we introduce a novel approach to compute bounds on the spectral gap and the spectral radius of the Laplacian matrix from a truncated sequence of Laplacian spectral moments. More explicitly, the problem solved in this section can be stated as follows:

Problem 1 (Moment-based bounds): Given a truncated sequence of Laplacian spectral moments $\left(m_k\left(L_{\mathcal{G}}\right)\right)_{k=1}^{K}$, find bounds on the spectral gap and the spectral radius of the Laplacian matrix $L_{\mathcal{G}}$.

In this section, we propose a solution to the above problem based on a recent result in [4]. In [4], Lasserre developed an approach to find bounds on the support of an unknown density function when only a sequence of its moments is available. In order to adapt Problem 1 to this framework, we need to introduce some definitions. Given a simple connected graph $\mathcal{G}$ with Laplacian eigenvalues $\{\lambda_i\}_{i=1}^n$, we define the *spectral density* of the nontrivial eigenvalue spectrum as

$$\rho_{\mathcal{G}}(\lambda) \triangleq \frac{1}{n-1} \sum_{i \geq 2} \delta(\lambda - \lambda_i), \tag{5}$$

where $\delta(\cdot)$ is the Dirac delta function. Notice how we have excluded the trivial eigenvalue, $\lambda_1 = 0$, from the spectral density; hence, the support [2] of $\rho_{\mathcal{G}}(\lambda)$ is equal to $supp(\rho_{\mathcal{G}}) = \{\lambda_i\}_{i=2}^n$. The moments of the spectral density in (5), denoted by $\overline{m}_k(L_{\mathcal{G}})$, can be written in terms of the spectral moments of $L_{\mathcal{G}}$, as follows

$$\begin{aligned} \overline{m}_k(L_{\mathcal{G}}) &\triangleq \int_{\mathbb{R}} \lambda^k \frac{1}{n-1} \sum_{i=2}^n \delta(\lambda - \lambda_i) \ d\lambda \\ &= \frac{1}{n-1} \sum_{i=2}^n \lambda_i^k = \frac{n}{n-1} m_k(L_{\mathcal{G}}), \end{aligned} \tag{6}$$

for all $k \geq 1$ (where we have used the fact that $\lambda_1 = 0$, in our derivations).

In what follows, we propose a solution to Problem 1 using a technique proposed by Lasserre in [4]. In that paper, the following problem was addressed:

Problem 2: Consider a truncated sequence of moments $(M_k)_{1 \leq r \leq K}$ corresponding to an unknown density function $\mu(\lambda)$, i.e., $M_k \triangleq \int \lambda^k d\mu(\lambda)$. Denote by $[a, b]$ the smallest interval containing the support of μ. Compute an upper bound $\alpha \geq a$ and a lower bound $\beta \leq b$ when only the truncated sequence of moments is available.

In the context of Problem 1, we have access to a truncated sequence of five spectral moments, $(m_k(L_{\mathcal{G}}))_{1 \leq k \leq 5}$, corresponding to the unknown spectral density function $\rho_{\mathcal{G}}$ and given by the expressions (2), (4), and (6). In this context, the smallest interval $[a, b]$ containing $supp(\rho_{\mathcal{G}})$ is equal to $[\lambda_2, \lambda_n]$. Therefore, a solution to Problem 2 would directly provide an upper bound on the spectral gap, $\alpha \geq \lambda_2$, and a lower bound on the spectral radius, $\beta \leq \lambda_n$. We now describe a numerical scheme proposed in [4] to solve Problem 2. This solution is based on a series of semidefinite programs in one variable. In order to formulate this series of SDP's, we need to introduce some definitions. For any $s \in \mathbb{N}$, let us consider a truncated sequence of moments

[2]Recall that the support of a density function μ on $\mathbb{R}$, denoted by $supp(\mu)$, is the smallest closed set B such that $\mu(\mathbb{R} \backslash B) = 0$.

$\mathbf{M} = (M_k)_{k=1}^{2s+1}$, associated with an unknown density function μ. We define the following Hankel matrices of moments:

$$R_{2s}(\mathbf{M}) \triangleq \begin{bmatrix} 1 & M_1 & \cdots & M_s \\ M_1 & M_2 & \cdots & M_{s+1} \\ \vdots & \vdots & \ddots & \vdots \\ M_s & M_{s+1} & \cdots & M_{2s} \end{bmatrix}, \; R_{2s+1}(\mathbf{M}) \triangleq \begin{bmatrix} M_1 & M_2 & \cdots & M_{s+1} \\ M_2 & M_3 & \cdots & M_{s+2} \\ \vdots & \vdots & \ddots & \vdots \\ M_{s+1} & M_{s+2} & \cdots & M_{2s+1} \end{bmatrix}. \quad (7)$$

We also define the *localizing matrix*[3] $H_s(x, \mathbf{M})$ as,

$$H_s(x, \mathbf{M}) \triangleq R_{2s+1}(\mathbf{M}) - x \; R_{2s}(\mathbf{M}). \quad (8)$$

Using the above matrices, Lasserre proposed in [4] the following series of SDP's to find a solution for Problem 2:

Solution to Problem 2: Let $\mathbf{M} = (M_k)_{k=1}^{2s+1}$ be a truncated sequence of moments associated with an unknown density function μ. Then

$$a \leq \alpha_s(\mathbf{M}) \triangleq \max_x \{x : H_s(x, \mathbf{M}) \succeq 0\}, \quad (9)$$

$$b \geq \beta_s(\mathbf{M}) \triangleq \min_x \{x : -H_s(x, \mathbf{M}) \succeq 0\}, \quad (10)$$

where $[a, b]$ is the smallest interval containing the support of μ.

Therefore, we can directly apply the above result to solve Problem 1 by considering the sequence of moments $\overline{\mathbf{m}} \triangleq (\overline{m}_r(L_\mathcal{G}))_{r=1}^{2s+1} = (\frac{n}{n-1} m_r(L_\mathcal{G}))_{r=1}^{2s+1}$ in the statement of the solution to Problem 2. Since this sequence of moments corresponds to the spectral density $\rho_\mathcal{G}$, with support $\{\lambda_i\}_{i=2}^n$, the solutions in (9) and (10) directly provide the following bounds on the spectral radius and spectral gap:

Solution to Problem 1: Let $\overline{\mathbf{m}} \triangleq (\frac{n}{n-1} m_r(L_\mathcal{G}))_{r=1}^{2s+1}$ be a truncated sequence of (scaled) Laplacian spectral moments associated with a graph $\mathcal{G}$. Then the Laplacian spectral gap and spectral radius of $\mathcal{G}$ satisfy the following bounds:

$$\lambda_2 \leq \alpha_s(\overline{\mathbf{m}}) \triangleq \max_x \{x : H_s(x, \overline{\mathbf{m}}) \succeq 0\}, \quad (11)$$

$$\lambda_n \geq \beta_s(\overline{\mathbf{m}}) \triangleq \min_x \{x : -H_s(x, \overline{\mathbf{m}}) \succeq 0\}. \quad (12)$$

[3] A more general definition of localizing matrix can be found in [**?**]. For simplicity, we restrict our definition to the particular form used in our problem.

In Section II, we derived expressions for the first five Laplacian spectral moments, $(m_r(L_{\mathcal{G}}))_{r=1}^5$, in terms of structural features of the network, namely, the degree sequence, the number of triangles, quadrangles and pentagons, and the correlation terms in (3). Therefore, we can apply the *Solution to Problem 1* to find bounds on λ_2 and λ_n.

In this section, we have presented an optimization-based approach to compute optimal bounds on the Laplacian spectral gap and spectral radius from a truncated sequence of Laplacian spectral moments. The truncated sequence of spectral moments $(m_k(L_{\mathcal{G}}))_{k=1}^5$ can be written in terms of local structural measurements using (2) and (4). Hence, the above methodology allows to compute bounds on the spectral radius and spectral gap of the Laplacian matrix given a collection of local structural features of the network. In the following section, we illustrate the usage of this approach with numerical examples.

IV. Structural Analysis and Simulations

In this section, we apply the moment-based approach herein proposed to study the relationship between structural and spectral properties of an unweighted, undirected graph representing the structure of the high-voltage transmission network of Spain (the adjacency of this network is available, in MATLAB format, in [8]). The number of nodes (buses) and edges (transmission lines) in this network are $n = 98$ and $e = 175$, respectively. From this dataset, we compute the set of structural properties involved in (2) and (4), namely, the power-sums of the degrees $(S_r)_{r=1}^5 = (350, 1692, 9836, 64056, 44942)$, the number of cycles $\Delta = 79$, $Q = 134$, $P = 232$, and the correlation terms $C_{dd} = 42.58$, $C_{d^2d} = 249.41$, $C_{dt} = 13.98$, $C_{d^2t} = 88.69$, $C_{dq} = 33.11$, and $D_{dd} = 80.77$. Using this collection of structural measurements, we use (2) and (4) to compute the first five Laplacian spectral moments of the Spanish transmission network: $(m_k(L_{\mathcal{G}}))_{k=1}^5 = (3.571, 20.83, 147.33, 1155.5, 9686.6)$. Using this sequence of spectral moments and the methodology described in Section III, we compute bounds on the spectral gap and spectral radius, α_2 and β_2, solving the SDP's in (11) and (12). The numerical values for these bounds, as well as the exact values for the spectral gap and spectral radius are: $\beta_2 = 9.18 \leq \lambda_n = 10.66$ and $\lambda_2 = 0.077 \leq \alpha_2 = 0.86$.

Our numerical analysis reveals that the Laplacian spectral radius and spectral moments of the electrical transmission network are strongly constrained by local structural features of the network. On the other hand, the spectral gap cannot be efficiently bounded using local structural features only, since the spectral gap strongly depends on the global connectivity of the network. This limitation is inherent to all spectral bounds based on local structural properties (see [9] for a wide collection of spectral bounds). In the following example, we illustrate this limitation with a simple example.

Example 4.1: Consider a ring graph with $n = 12$ nodes, which we denote by R_{12}. The eigenvalues of the Laplacian matrix of a ring graph of length l, R_l, are equal to $\lambda_i = 2 - 2\cos(2\pi i/l)$, for $i = 0, ..., l-1$ [5]. Therefore, the Laplacian spectral gap and spectral radius of R_{12} are $\lambda_2 = 2 - 2\cos\pi/6 \approx 0.2679$ and $\lambda_n = 4$, respectively. We can also compute the moment-based bounds α_2 and β_2 using local structural measurements, as follows. The degrees of all the nodes in R_{12} are $d_i = 2$; thus, the power sums of the degrees are equal to $S_k = 2^k 12$. The number of triangles, quadrangles and pentagons are $\Delta = Q = P = 0$. The correlation terms are $C_{dd} = 4$, $C_{d^2d} = 8$, and the rest of correlation terms in (3) are equal to zero. Based on these structural measurements, we have from (2) and (4) that the first five Laplacian spectral moments are $(m_r(L_{\mathcal{G}}))_{r=1}^5 = (2, 6, 20, 70, 252)$, and the resulting moment-based bounds from (11) and (12) are $\beta_2 = 3.732 \leq 4$ and $\alpha_2 = 0.2679 \approx \lambda_2$. Therefore, both the bounds on the spectral radius and the spectral gap are very tight for R_{12}. In particular, α_2 is remarkably close to λ_2.

On the other hand, we can construct graphs with the same local structural properties (and, therefore, the same first five spectral moments, and bounds α_2 and β_2), but very different spectral gap, as follows. Consider a graph of 12 nodes consisting in two disconnected rings of length 6. It is easy to verify that this (disconnected) graph presents the same local structural features as a connected ring of length 12, namely, the degrees of all the nodes are $d_i = 0$, the number of cycles $\Delta = Q = P = 0$, and the correlation terms are the same as the ones computed above. In contrast to R_{12}, the spectral gap of this disconnected graph is equal to zero, $\lambda_2 = 0$, which is very different than the moment-based bound α_2.

In general, the Laplacian spectral gap is a global property that quantifies how 'well-connected' a network is [10]. Since the structural measurements used in our bounds (degree sequence, correlation terms, etc.) have a local nature, they do not contain enough information to determine how well connected the network is globally. In other words, it is often possible to find two different graphs with identical local structural features but radically different global structure, as we have illustrated in the above example.

V. Conclusions

This paper studies the relationship between *local* structural features of large complex networks and *global* spectral properties of their Laplacian matrices. In Section II, we have proposed a graph-theoreical approach to compute the first five Laplacian spectral moments of a network from a collection of local structural measurements. In Section III, we have proposed an optimization-based approach, based on a recent result by Lasserre [4], to compute bounds on the Laplacian spectral radius and spectral gap of a network from a truncated sequence of spectral moments. Our bounds take into account the effect of important structural properties that are usually neglected in most of the bounds found in the literature, such as the distribution of cycles and other structural correlations. Our analysis shows that local structural features of the network strongly constrain the Laplacian spectral moments and spectral radius. On the other hand, local structural features are not enough to characterize the Laplacian spectral gap, since this quantity strongly depends on how 'well-connected' the network is globally.

Appendix

Theorem 2.3 Let $\mathcal{G}$ be a simple graph with Laplacian matrix $L_{\mathcal{G}}$. Then, the fourth and fifth Laplacian moments can be written as

$$\begin{aligned} m_4\left(L_{\mathcal{G}}\right) &= \frac{1}{n}\left(-S_1+2S_2+4S_3+S_4+8Q\right) \\ &\quad +4C_{dd}-8C_{dt}, \\ m_5\left(L_{\mathcal{G}}\right) &= \frac{1}{n}\left(-5S_2+5S_3+5S_4+S_5+30\Delta-10P\right) \\ &\quad +10\left(C_{dd}+C_{d^2d}-C_{dt}-C_{d^2t}+C_{dq}-D_{dd}\right) \end{aligned}$$

where $S_r=\sum_{v_i\in\mathcal{V}} d_i^r$, and the correlation terms C_{dd}, C_{dt}, C_{dq}, C_{d^2d}, C_{d^2t}, and D_{dd} are defined in (3).

Proof: As in Theorem 2.2, we use Lemma 2.1 to compute the Laplacian spectral moments in terms of weighted sums of closed walks in the weighted Laplacian graph $\mathcal{L}_G$. In order to compute the fourth Laplacian spectral moment, we classify the types of possible closed walks of length 4 into subsets according to the structure of the underlying graph covered by the walk. Specifically, two walks p_1 and p_2 belong to the same type if the subgraphs covered by the walks, denoted by $C\left(p_1\right)$ and $C\left(p_2\right)$ according to Definition 2.2, are isomorphic. We enumerate

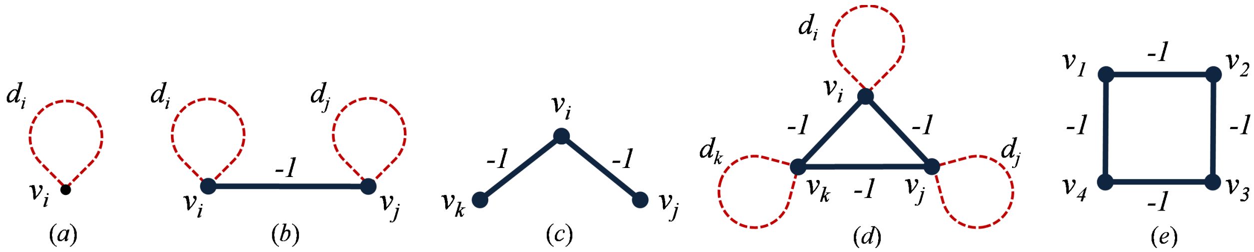

Fig. 1. Collection of possible graphs covered by closed walks of length 4.

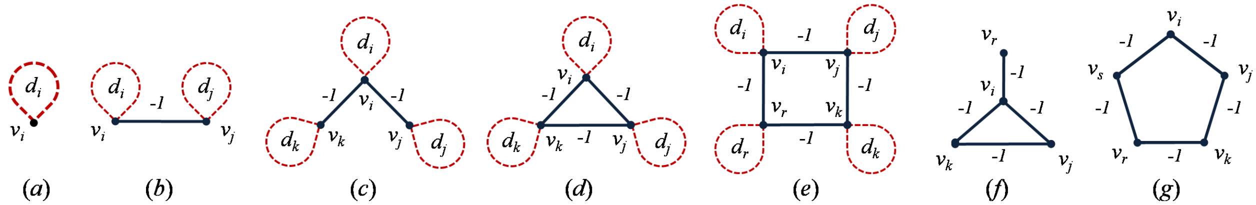

Fig. 2. Collection of possible graphs covered by closed walks of length 5.

the possible types in Fig. 1 and we denote the corresponding sets of walks as $P_{4a}^{(i)}$, $P_{4b}^{(i)}$, $P_{4c}^{(i)}$, $P_{4d}^{(i)}$, and $P_{4e}^{(i)}$. These sets $P_{4a}^{(i)}$,...,$P_{4e}^{(i)}$ partition the set of closed walks $P_{4,n}^{(i)}$. Hence, we have $m_4\left(L_{\mathcal{G}}\right) = \frac{1}{n}\sum_{v_i\in\mathcal{V}}\sum_{x\in\{a,b,c,d,e\}}\sum_{p\in P_{4x}^{(i)}}\omega\left(p\right).$

We now analyze each one of the terms in the above summations. For convenience, we define $T_{4x} \triangleq \frac{1}{n}\sum_{v_i\in\mathcal{V}}\sum_{p\in P_{4x}^{(i)}}\omega\left(p\right),$ and analyze the term T_{4x} for $x\in\{a,b,c,d\}$:

(a) For $x=a$, we have that the weights $\omega\left(p\right)$ of the walks in $P_{4a}^{(i)}$ are all the same, and equal to d_i^4. Hence, $T_{4a}=\frac{1}{n}\sum_i d_i^4 = S_4/n$.

(b) For $x=b$, the weights of the walks in $P_{4b}^{(i)}$ are equal to $2+4\left(d_i^2+d_j^2+d_id_j\right)$. Hence, $T_{4b}=\frac{1}{n}\sum_{v_i\sim v_j}2+4\left(d_i^2+d_j^2+d_id_j\right)=\frac{1}{n}\left(S_1+4S_3\right)+4C_{dd}$.

(c) For $x=c$, the weights of the walks in $P_{4c}^{(i)}$ (i.e., walks that cover the two-chain graph) are equal to 4. Hence, $T_{4c}=\frac{1}{n}\sum_{v_j\sim v_i\sim v_k}4 \overset{(i)}{=} \frac{1}{n}\sum_{i=1}^{n}\binom{d_i}{2}4=\frac{2}{n}\left(S_2-S_1\right),$ where in equality (i) we have used the fact that the number of two-chain graphs whose center node is v_i is equal to $\binom{d_i}{2}$.

(d) For $x=d$, the weights of the walks in $P_{4d}^{(i)}$ are equal to $-8\left(d_i+d_j+d_k\right)$. Hence, $T_{4d}=\frac{1}{n}\sum_{v_i\sim v_j\sim v_k\sim v_i}-8\left(d_i+d_j+d_k\right)=-\frac{8}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}3t_{ijk}d_i$,where t_{ijk} is an indicator function that takes value 1 if $v_i\sim v_j\sim v_k\sim v_i$. Since $\sum_{j=1}^{n}\sum_{k=1}^{n}3t_{ijk}=t_i$ (the number of triangles touching node v_i), we have that $T_{4d}=-\frac{8}{n}\sum_{i=1}^{n}t_id_i=-8C_{dt}$.

(e) For $x=e$, the weights of the walks in $P_{4e}^{(i)}$ are equal to 8. Hence, $T_{4e}=\frac{1}{n}\sum_{\substack{v_i\sim v_j\sim v_k\sim v_r\sim v_i\\ \text{s.t. } 1\leq i<j<k<r\leq n}} 8 = 8Q/n$.

Finally, since $m_4\left(L_{\mathcal{G}}\right)=T_{4a}+T_{4b}+T_{4c}+T_{4d}$, we obtain the expression for the fourth Laplacian spectral moment in the statement of the theorem after simple algebraic simplifications.

In order to derive a similar expression for the fifth-order Laplacian spectral moments, we follow an identical approach. Below, we provide the main steps in the derivations. As before, we partition the set of closed walks $P_{5,n}^{(i)}$ according to the subgraph covered by the walk. We show the structure of the possible subgraphs in Fig. 2.

We now analyze each one of the terms $T_{5x}\triangleq\frac{1}{n}\sum_{v_i\in\mathcal{V}}\sum_{p\in P_{5x}^{(i)}}\omega\left(p\right)$ for $x\in\{a,b,...,g\}$:

(a) For $x=a$, we have $T_{5a}=\frac{1}{n}\sum_{i=1}^{n}d_i^5=S_5/n$.

(b) For $x=b$, we can determine all possible closed walks of length 5 using the edge graph in Fig. 2(b) and derive that $T_{5b}=\frac{1}{n}\sum_{v_i\sim v_j}5\left(d_i+d_j+d_i^3+d_j^3+d_i^2d_j+d_id_j^2\right)=\frac{5}{n}\left(S_2+S_4\right)+10C_{d^2d}$.

(c) For $x=c$, the weights of walks covering the two-chain graph are d_i, d_j, d_k. Counting the multiplicities of each type of walk, we have that $T_{5c}=\frac{1}{n}\sum_{v_j\sim v_i\sim v_k}10d_i+5d_j+5d_k=\frac{10}{n}\sum_{i=1}^{n}\binom{d_i}{2}d_i+\frac{5}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij}\left(d_i-1\right)d_j$,where we have used that $\sum_{v_i\sim v_j\sim v_k}d_i=\sum_{i=1}^{n}\binom{d_i}{2}d_i$ and $\sum_{v_j\sim v_i\sim v_k}d_j=\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij}\left(d_i-1\right)d_j$. Thus, $T_{5c}=\frac{5}{n}\sum_{i=1}^{n}d_i^3-\frac{5}{n}\sum_{i=1}^{n}d_i^2+\frac{5}{n}\sum_{1\leq i,j\leq n}a_{ij}d_id_j-\frac{5}{n}\sum_{j=1}^{n}d_j^2=\frac{5}{n}\left(S_3-2S_2\right)+10C_{dd}$

(d) For $x=d$, we can determine all possible closed walks of length 5 using the edge graph in Fig. 2(d) and derive that where $b_{ij}\triangleq\sum_{k=1}^{n}a_{ik}a_{jk}=\left|\mathcal{N}_i\cap\mathcal{N}_j\right|$, the number of common neighbors shared by v_i and v_j. Hence, $T_{5d}=-\frac{30\Delta}{n}-\frac{10}{n}\sum_{i=1}^{n}t_id_i^2-\frac{10}{n}\sum_{i\sim j}a_{ij}b_{ij}\left(d_id_j\right)=-30\Delta/n-10C_{d^2t}-10D_{dd}$

(e) For $x=e$, the weights of walks covering the quadrangle graph are d_i, d_j, d_k, and d_r. Counting the multiplicities of each type of walk we have that $T_{5e}=\frac{1}{n}\sum_{v_i\sim v_j\sim v_k\sim v_r\sim v_i}10\left(d_i+d_j+d_k+d_r\right)=\frac{10}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{r=1}^{n}4q_{ijkr}d_i$,where q_{ijkr} is an indicator function that takes value 1 if $v_i\sim v_j\sim v_k\sim v_r\sim v_i$. Since $\sum_{1\leq j,k,r\leq n}4q_{ijkr}=q_i$ (the number of quadrangles touching node v_i), we have that $T_{5e}=\frac{10}{n}\sum_{i=1}^{n}q_id_i=10C_{dq}$.

(f) For $x=f$, we have 10 possible walks covering the subgraph in Fig. 2(f). Since each walks has a weight equal to -1, we have that $T_{5f}=\frac{1}{n}\sum_{v_i\sim v_j\sim v_k\sim v_i\sim v_r}-10=-\frac{10}{n}\sum_{i=1}^{n}\left(d_i-2\right)t_i$, where in the last equality we take into account that the number of subgraphs of the type depicted in Fig. 2(f) and centered at node v_i is equal to the number of triangles touching node v_i,

t_i, multiplied by $(d_i - 2)$ (where we have subtracted -2 to the degree to discount the two edges touching v_i that are part of each triangle counted in t_i). Hence, we have that $T_{5f} = -\frac{10}{n}\sum_{i=1}^{n} d_i t_i + \frac{10}{n}\sum_{i=1}^{n} 2t_i = -10C_{dt} + 60\Delta/n$.

(g) For $x = f$, we have 10 possible walks on the pentagon and the associated weight of each walk is -1. Hence, $T_{5g} = \frac{1}{n}\sum_{v_i \sim v_j \sim v_k \sim v_r \sim v_s \sim v_i} -10 = -10P/n$,where P is the total number of pentagons in $\mathcal{G}$.

Finally, since $m_5\left(L_{\mathcal{G}}\right) = T_{5a} + T_{5b} + ... + T_{5g}$, we obtain the expression for the fifth Laplacian spectral moment in the statement of the theorem after simple algebraic simplifications. ■

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