# Structural Analysis of Laplacian Spectral Properties with Application to Electric Transmission Networks 

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#### Abstract

The spectrum of the Laplacian matrix of a network plays a key role in a wide range of dynamical problems associated with the network, from transient stability analysis of power networks to distributed control of formations. Using methods from algebraic graph theory and convex optimization, we study the relationship between structural features of a network and spectral properties of its Laplacian matrix. We illustrate our results by studying the influence of structural properties on the Laplacian eigenvalues of the American (western states), French and Spanish high-voltage transmission networks. Our study suggests that for such networks the Laplacian spectral radii and spectral moments are strongly constrained by a particular set of local structural features, namely the degree sequence and the so-called joint-degree distribution. On the other hand, other structural properties that may seem important, such as the distribution of cycles in the network, appear to have a very weak influence on the Laplacian spectrum of electrical transmission networks. We also show that local structural features are not enough to characterize the Laplacian spectral gap. Therefore, since the spectral gap is fundamental in the analysis of many dynamical processes on networks, random models in which only local structural features are prescribed are typically insufficient to generate synthetic topologies in which these dynamical processes can be studied.


## I. Introduction

The eigenvalue spectrum of the Laplacian matrix of a network provides valuable information regarding the behavior of many dynamical processes taking place on the network. In their seminal paper [1], Pecora and Carrol related the problem of synchronization in a network of coupled oscillators to the largest and second-smallest Laplacian eigenvalues of the network (usually denoted by Laplacian spectral radius and spectral gap, respectively). More recently, Dorfler and Bullo derived conditions for transient stability in power networks in terms of the spectral gap of the Laplacian matrix [2]. Apart from their applicability to the problems of synchronization and transient stability analysis, the Laplacian eigenvalues are also relevant in the analysis of many distributed estimation and control problems (see [3],[4] and references therein).

Understanding the relationship between the structure of a complex network and the behavior of dynamical processes taking place in it is a central question in the research field of

[^0]network science [5]. Since the behavior of many networked dynamical processes is closely related with the Laplacian eigenvalues [6], it is of interest to study the relationship between structural features of the network and its Laplacian eigenvalues. In this paper 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. Our analysis reveals that there are certain spectral properties, such as the spectral radius and the so-called spectral moments, that can be efficiently estimated from local structural features of the network.

The most common approach to study the relationship between structural and spectral properties of a network is by means of random network models. This approach has been widely used to study the effect of the degree distribution [7], correlations [8], or clustering [9], in a broad range of realworld networks. Although very common in the literature, this approach presents a serious drawback: when we prescribe the structural feature under study in the random network model, there are other structural features that are being indirectly induced in the network and may be relevant in the network's behavior. Since those induced features are not directly controlled, it is difficult (if not impossible) to isolate the role of the structural feature under study using random network models.

In this paper, we present a novel approach to study the influence of certain structural features on the network Laplacian eigenvalues without using random models. Our approach builds on algebraic graph theory and convex optimization to study relevant properties of the Laplacian spectrum. We apply our theoretical results in the study of real electrical transmission networks. In particular, we analyze high-voltage transmission networks in the USA (western states), France and Spain. Our numerical results show that, in the case of electrical transmission networks, the Laplacian spectral radii and spectral moments are strongly constrained by a particular set of local structural features: the degree distribution and the so-called joint-degree distribution. On the other hand, other structural properties that may seem important, such as the distribution of cycles in the network, appear to have a very weak influence on the Laplacian spectrum of electrical transmission networks. In our numerical experiments, we also verify that local structural features are not enough to characterize the Laplacian spectral gap, since this spectral property measures, to a certain extent, how well a network is globally connected. Therefore, since the spectral gap is fundamental
in the analysis of many dynamical processes on networks, random models in which only local structural features are prescribed, such as those in [7]-[9], are insufficient to generate synthetic topologies in which these dynamical processes can be studied.

The rest of this paper is organized as follows. In the next section, we define graph-theoretical terminology needed in our derivations. In Section III, we review some previous results relating the eigenvalues of the Laplacian matrix of a network to its structural features, and introduce a novel methodology based on algebraic graph theory to derive closedform expressions for the so-called Laplacian spectral moments. In Section IV, we use convex optimization to derive tight bounds on important properties of the Laplacian spectrum from the spectral moments. We apply our theoretical results to the analysis of the Laplacian spectra of the American (western states), French and Spanish high-voltage transmission networks in Section V

## II. Preliminaries

Let $\mathcal{G}=(\mathcal{V}, \mathcal{E})$ be an undirected graph, where $\mathcal{V}=$ $\left\{v_{1}, \ldots, v_{n}\right\}$ denotes a set of $n$ nodes and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ denotes a set of $e$ undirected edges. If $\left\{v_{i}, v_{j}\right\} \in \mathcal{E}$, 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 $\mathcal{N}_{i}=\left\{w \in \mathcal{V}:\left\{v_{i}, w\right\} \in \mathcal{E}\right\}$. The degree $d_{i}$ of a vertex $v_{i}$ is the number of nodes adjacent to it, i.e., $d_{i}=\left|\mathcal{N}_{i}\right|$. We consider three types of undirected graphs:
(i) A graph is called simple if its edges are unweighted and it has no self-loop $\mathbb{1}^{1}$.
(ii) A graph is loopy if it has self-loops.
(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 $\operatorname{triad} \mathcal{H}=(\mathcal{V}, \mathcal{E}, \mathcal{W})$, where $\mathcal{V}$ and $\mathcal{E}$ are the sets of nodes and edges in $\mathcal{H}$, and $\mathcal{W}=\left\{w_{i j} \in \mathbb{R}\right.$, for all $\left.\left\{v_{i}, v_{j}\right\} \in \mathcal{E}\right\}$ is the set of (possibly negative) weights.

Graphs can be algebraically represented via matrices. The adjacency matrix of a simple graph $\mathcal{G}$, denoted by $A_{\mathcal{G}}=\left[a_{i j}\right]$, is an $n \times n$ symmetric matrix defined entry-wise as $a_{i j}=1$ if nodes $v_{i}$ and $v_{j}$ are adjacent, and $a_{i j}=0$ otherwise. In the case of weighted graphs (and possibly non-simple), the weighted adjacency matrix is defined by $W_{\mathcal{G}}=\left[w_{i j}\right]$, where $w_{i j}=0$ if $v_{i}$ is not adjacent to $v_{j}$. We define the degree matrix of a simple graph $\mathcal{G}$ as the diagonal matrix $D_{\mathcal{G}}=\operatorname{diag}\left(d_{i}\right)$. 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 $L_{\mathcal{G}} \succeq 0$ [10]. Thus, $L_{\mathcal{G}}$ has a full set of $n$ real and orthogonal eigenvectors with real nonnegative eigenvalues $0=\lambda_{1} \leq \lambda_{2} \leq \ldots \leq \lambda_{n}$. Furthermore, the trivial eigenvalue $\lambda_{1}=0$ of $L_{\mathcal{G}}$ always admits a corresponding eigenvector $v_{1}=(1,1, \ldots, 1)^{T}$. The algebraic multiplicity of the trivial eigenvalue is equal to the number of connected components

[^1]in $\mathcal{G}$, which we assume to be equal to one in the rest of the paper. The smallest and largest nontrivial eigenvalues of $L_{\mathcal{G}}$, $\lambda_{2}$ and $\lambda_{n}$, are called the spectral gap and spectral radius of $L_{\mathcal{G}}$, respectively, and they play an important role in this paper. Given a $n \times n$ real and symmetric matrix $B$ with (real) eigenvalues $\sigma_{1}, \ldots, \sigma_{n}$, 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 III-B, there is an interesting connection between the spectral moments of the Laplacian matrix, $m_{k}\left(L_{\mathcal{G}}\right)$, and structural features of the graph.

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, $\left(d_{1}, \ldots, d_{n}\right)$. The $p$-th power-sum of the degree sequence is defined as

$$
\begin{equation*}
S_{p} \triangleq \sum_{v_{i} \in \mathcal{V}} d_{i}^{p} \tag{1}
\end{equation*}
$$

A walk of length $k$ from $v_{i_{1}}$ to $v_{i_{k+1}}$ is an ordered sequence of nodes $\left(v_{i_{1}}, v_{i_{2}}, \ldots, v_{i_{k+1}}\right)$ such that $v_{i_{j}} \sim v_{i_{j+1}}$ for $j=$ $1,2, \ldots, k$. 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 $p=\left(v_{i_{1}}, v_{i_{2}}, \ldots, v_{i_{k+1}}\right)$ in a weighted graph $\mathcal{H}$, we define the weight of the walk as, $\omega(p)=w_{i_{1} i_{2}} w_{i_{2} i_{3}} \ldots w_{i_{k} i_{k+1}}$.

Finally, we define the concept of local neighborhood around a node. Let $\delta\left(v_{i}, v_{j}\right)$ denote the distance between two nodes $v_{i}$ and $v_{j}$ (i.e., the minimum length of a walk from $v_{i}$ to $v_{j}$ ). We say that $v_{i}$ and $v_{j}$ are $r$-th neighbors if $\delta\left(v_{i}, v_{j}\right)=r$, and define the $r$-th order neighborhood around $v_{i}$ as the set of nodes $\mathcal{N}_{i}^{(r)} \triangleq\left\{w \in \mathcal{V}: \delta\left(v_{i}, w\right) \leq r\right\}$. By convention, we assume that $\delta(v, v)=0$, hence, the first-order neighborhood of $v_{i}$ satisfies $\mathcal{N}_{i}^{(1)}=\mathcal{N}_{i} \cup v_{i}$. The nodes in $\mathcal{N}_{i}^{(r)}$ induce an (unlabeled) local subgraph $\mathcal{G}_{i}^{(r)}=\left(\mathcal{N}_{i}^{(r)}, \mathcal{E}_{i}^{(r)}\right) \subseteq \mathcal{G}$, where $\mathcal{E}_{i}^{(r)}=\left\{\{v, w\} \in \mathcal{E}\right.$ s.t. $\left.v, w \in \mathcal{N}_{i}^{(r)}\right\}$, i.e., the set of edges connecting nodes in $\mathcal{N}_{i}^{(r)}$. It is worth remarking that these local subgraphs are unlabeled; thus, it is impossible, in general, to reconstruct the complete network $\mathcal{G}$ from the set of local subgraphs $\left\{\mathcal{G}_{i}^{(r)}, i=1, \ldots, n\right\}$. These subgraphs are useful to define the concept of local structural measurement. We say that a structural measurement is local with a certain radius $r$ if it can be computed from the set of local subgraphs $\left\{\mathcal{G}_{i}^{(r)}\right.$, $i=1, \ldots, n\}$. For example, the degree sequence of a graph is a local structural measurement (with radius 1), since we can compute the degree of each node $v_{i}$ from the local subgraph $\mathcal{N}_{i}^{(1)}$. Similarly, one can compute the number of triangles touching $v_{i}$ from $\mathcal{N}_{i}^{(1)}$; hence, the total number of triangles in $\mathcal{G}$ is a local measurement with radius 1 . In contrast, the eigenvalue spectrum of the Laplacian matrix is not a local property, since we cannot compute the eigenvalues unless we know the complete graph structure. One of the main contributions of this paper is to propose a novel methodology to extract global information regarding the Laplacian eigenvalue spectrum from local structural measurements of the network.

## III. Spectral Analysis of the Laplacian Matrix

The spectrum of the Laplacian matrix is relevant in a wide range of networked dynamical processes, such as synchronization of coupled oscillators [1], flocking and formation control of multi-agent systems [3],[4], or distributed consensus algorithms [11]. In the context of power networks, Laplacian eigenvalues contain useful information for the analysis of synchronization and transient stability [2]. Among the Laplacian eigenvalues, the spectral radius and the spectral gap are specially important in dynamical applications and we pay particular attention to them.

In this paper we introduce a novel approach to study the effect of structural properties of a network on the spectrum of its Laplacian matrix, by using the moments of the eigenvalue distribution. Before we introduce our approach, we first review some of the most relevant known bounds on the Laplacian eigenvalues.

## A. Bounds on Laplacian Eigenvalues

The literature contains a large collection of upper and lower bounds on the spectral gap $\lambda_{2}$ and the spectral radius $\lambda_{n}$ in terms of structural features of a network, such as degree distributions. Let us consider a simple graph $\mathcal{G}$ with $n$ nodes, $e$ edges, and degree sequence $\left(d_{i}\right)_{i=1}^{n}$. Let $m_{i}$ be the average degree of the neighbors of $v_{i}$, i.e., $m_{i} \triangleq \frac{1}{d_{i}} \sum_{v_{j} \in \mathcal{N}_{i}} d_{j}$ (note that $m_{i}$ is a local structural measurement with radius 2). For connected networks, we have the following upper and lower bounds on the Laplacian spectral gap in terms of local structural measurements (see [12] for an extensive review):

$$
\begin{aligned}
& \lambda_{2} \geq\left(\frac{(n-1) \bar{m}}{2}-\frac{n-2}{4}\right)^{-1}, \text { from [13] } \\
& \lambda_{2} \leq \kappa_{e} \leq \min _{v_{i} \in \mathcal{V}}\left\{d_{i}\right\}, \text { from [14], }
\end{aligned}
$$

where $\bar{m} \triangleq \frac{1}{n} \sum_{v_{i} \in \mathcal{V}} m_{i}$ and $\kappa_{e}$ is the edge connectivity $\left.\right|^{2}$ of the graph. Although many other bounds can be found in the literature, most of them involve properties that cannot be computed from local structural features of the network, such as the diameter of the network or the average distance between every pair of nodes [12]. Since the spectral gap strongly depends on the global connectivity of the network, bounds on the spectral gap written in terms of local structural features usually perform poorly in practice (as we shall verify in Section V.

Similarly, we find in the literature a large variety of upper and lower bounds on the Laplacian spectral radius $\lambda_{n}$ (see, for example, [15] for a collection of bounds). Many of these bounds can be written as the maximum or minimum of certain functions defined over the set of nodes or edges. For example,

$$
\begin{aligned}
\lambda_{n} & \leq \max _{\left\{v_{i}, v_{j}\right\} \in \mathcal{E}} \frac{d_{i}+d_{j}+\sqrt{\left(d_{i}-d_{j}\right)^{2}+4 m_{i} m_{j}}}{2}, \\
\lambda_{n} & \geq \sqrt{2} \min _{v_{i} \in \mathcal{V}}\left(d_{i}^{2}+d_{i} m_{i}\right)^{1 / 2},
\end{aligned}
$$

[^2]As we shall verify in Section $V$, the above upper bound on the spectral radius is quite tight in the case of electrical transmission networks, while lower bounds found in the literature are very loose. In Section IV, we shall derive lower bounds that outperform those found in the literature in the case of electrical transmission networks.

## B. Moment-Based Analysis of the Laplacian Spectrum

In this section, we use algebraic graph theory to relate spectral properties of a network to a rich variety of local structural measurements. First, we need to introduce some preliminary results and concepts. A well-known result in algebraic graph theory relates the diagonal entries of the $k$ th power of the adjacency matrix, $\left[A_{\mathcal{G}}^{k}\right]_{i i}$, to the number of closed walks of length $k$ in $\mathcal{G}$ that start and finish at node $v_{i}$ [10]. 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 $W_{\mathcal{H}}=\left[w_{i j}\right]$. Then

$$
\left[W_{\mathcal{H}}^{k}\right]_{i i}=\sum_{p \in P_{k, n}^{(i)}} \omega(p)
$$

where $P_{k, n}^{(i)}$ is the set of closed walks of length $k$ from $v_{i}$ to itself in the complete loopy graph ${ }^{3}$ and $\omega(p)$ is the weight of walk $p$ in $\mathcal{H}$.

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

$$
\begin{equation*}
\left[W_{\mathcal{H}}^{k}\right]_{i i}=\sum_{i=1}^{n} \sum_{i_{2}=1}^{n} \cdots \sum_{i_{k}=1}^{n} w_{i, i_{2}} w_{i_{2}, i_{3}} \cdots w_{i_{k}, i} \tag{2}
\end{equation*}
$$

Using the graph-theoretic nomenclature introduced in Section II. we have that $w_{i, i_{2}} w_{i_{2}, i_{3}} \ldots w_{i_{k}, i}=\omega(p)$, for $p=$ $\left(v_{i}, v_{i_{2}}, v_{i_{3}}, \ldots, v_{i_{k}}, v_{i}\right)$. Hence, the summations in 2) can be written as $\left[W_{\mathcal{H}}^{k}\right]_{i i}=\sum_{1 \leq i, i_{2}, \ldots, i_{k} \leq n} \omega(p)$. Finally, the set of closed walks $p=\left(v_{i}, v_{i_{2}}, v_{i_{3}}, \ldots, v_{i_{k}}, v_{i}\right)$ with indices $1 \leq i, i_{2}, \ldots, i_{k} \leq n$ is equal to the set of closed walks of length $k$ from $v_{i}$ to itself in the complete loopy graph $J_{n}$ (which we have denoted by $P_{k, n}^{(i)}$ in the statement of the Proposition).

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

Lemma 3.1: Let $\mathcal{H}=(\mathcal{V}, \mathcal{E}, \mathcal{W})$ be a weighted graph with weighted adjacency matrix $W_{\mathcal{H}}=\left[w_{i j}\right]$. Then

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

where $P_{k, n}^{(i)}$ is the set of closed walks of length $k$ from $v_{i}$ to itself in the complete loopy graph $J_{n}$.

[^3]

Fig. 1. A simple graph $\mathcal{G}_{4}$ (left) and its corresponding Laplacian weighted graph $\mathcal{L}\left(\mathcal{G}_{4}\right)$ (right).

Proof: Let us denote by $\mu_{1}, \ldots, \mu_{n}$ the set of (real) eigenvalues of the (symmetric) weighted adjacency matrix $W_{\mathcal{H}}$. We have that the moments can be written as

$$
m_{k}\left(W_{\mathcal{H}}\right) \triangleq \frac{1}{n} \sum_{i=1}^{n} \mu_{i}^{k}=\frac{1}{n} \operatorname{Trace}\left(W_{\mathcal{H}}^{k}\right)
$$

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

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

In Subsections III-B1 and III-B2, we shall apply this result to compute the spectral moments of the Laplacian matrix in terms of local structural measurements. First, we need to introduce a weighted graph that is useful in our derivations:

Definition 3.1: Given a simple graph $\mathcal{G}=(\mathcal{V}, \mathcal{E})$, we define the Laplacian graph of $\mathcal{G}$ as the weighted graph $\mathcal{L}(\mathcal{G}) \triangleq\left(\mathcal{V}, \mathcal{E} \cup \mathcal{S}_{n}, \Gamma\right)$, where $\mathcal{S}_{n}=\{\{v, v\}$ for all $v \in \mathcal{V}\}$ (the set of all self-loops), and $\Gamma=\left[\gamma_{i j}\right]$ is a set of weights defined as:

$$
\gamma_{i j} \triangleq \begin{cases}-1, & \text { for }\left\{v_{i}, v_{j}\right\} \in \mathcal{E} \\ d_{i}, & \text { for } i=j \\ 0, & \text { otherwise }\end{cases}
$$

Remark 3.1: 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 3.1 to express the spectral moments of the Laplacian matrix $L_{\mathcal{G}}$ in terms of weighted walks in the Laplacian graph $\mathcal{L}(\mathcal{G})$.
Example 3.1: In Fig. 1(a) we have a simple graph with 4 nodes, $\mathcal{G}_{4}$. In Fig. 1(b) we have its corresponding Laplacian weighted graph $\mathcal{L}\left(\mathcal{G}_{4}\right)$. Observe how the edges in $\mathcal{G}_{4}$ are also edges in $\mathcal{L}\left(\mathcal{G}_{4}\right)$ with an associated weight of -1 . Also, each node in $\mathcal{L}\left(\mathcal{G}_{4}\right)$ presents a self-loop with a weight equal to the degree of the corresponding node in $\mathcal{G}_{4}$. One can easily check that the Laplacian matrix of $\mathcal{G}_{4}$ is equal to the weighted adjacency matrix of $\mathcal{L}\left(\mathcal{G}_{4}\right)$.

Before we apply Lemma 3.1 to study the Laplacian spectral moments, we must introduce the concept of subgraph covered by a walk.

Definition 3.2: Consider a walk $p=\left(v_{i_{1}}, v_{i_{2}}, \ldots, v_{i_{k+1}}\right)$ of length $k$ in a (possibly loopy) graph. We define the subgraph
covered by $p$ as the simple graph $C(p)=\left(\mathcal{V}_{c}(p), \mathcal{E}_{c}(p)\right)$, with node-set $\mathcal{V}_{c}(p)=\bigcup_{r=1}^{k+1} v_{i_{r}}$, and edge-set

$$
\mathcal{E}_{c}(p)=\bigcup_{v_{i_{r}} \neq v_{i_{r+1}}}\left\{v_{i_{r}}, v_{i_{r+1}}\right\}, \text { for } 1 \leq r \leq k+1
$$

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 3.2 For example, consider a walk $p=\left(v_{1}, v_{2}, v_{2}, v_{3}, v_{3}, v_{1}, v_{3}, v_{1}\right)$ in a graph with self-loops. Then, $C(p)$ has node-set $\mathcal{V}_{c}(p)=\left\{v_{1}, v_{2}, v_{3}\right\}$ and edge-set $\mathcal{E}_{c}(p)=\left\{\left\{v_{1}, v_{2}\right\},\left\{v_{2}, v_{3}\right\},\left\{v_{3}, v_{1}\right\}\right\}$. In other words, $C(p)$ is a simple triangle.

In the following subsections, we build on Lemma 3.1 to derive closed-form expressions for a sequence of Laplacian spectral moments in terms of relevant structural features of the network. In Subsection III-B1, we provide expressions for the first three spectral moments in terms of the degree sequence and the number of triangles in $\mathcal{G}$. In Subsection III-B2, we compute higher-order moments in terms of longer cycles and more elaborate structural measurements.

1) Low-Order Laplacian Spectral Moments: In this subsection we derive expressions for the first three spectral moments of the Laplacian matrix of a simple graph using graphtheoretical concepts.

Theorem 3.2: Let $\mathcal{G}$ be a simple graph with Laplacian matrix $L_{\mathcal{G}}$. Then, the first three spectral moments of the Laplacian matrix are

$$
\begin{align*}
m_{1}\left(L_{\mathcal{G}}\right) & =\frac{1}{n} S_{1}  \tag{3}\\
m_{2}\left(L_{\mathcal{G}}\right) & =\frac{1}{n}\left(S_{1}+S_{2}\right) \\
m_{3}\left(L_{\mathcal{G}}\right) & =\frac{1}{n}\left(3 S_{2}+S_{3}-6 \Delta\right)
\end{align*}
$$

where $S_{p}$ is defined in (1), and $\Delta$ is the total number of triangles in $\mathcal{G}$.

Proof: First, we apply Lemma 3.1 to compute the Laplacian spectral moments of a simple graph $\mathcal{G}$ in terms of closed walks in the weighted Laplacian graph $\mathcal{L}(\mathcal{G})$, described in Definition 3.1. In particular, the first spectral moment is related to the set of closed walks of length 1 . Clearly, the only possible closed walks of length 1 in $\mathcal{L}(\mathcal{G})$ are those using a self-loop, i.e., $P_{1, n}^{(i)}=\left\{\left(v_{i}, v_{i}\right)\right.$ for $\left.v_{i} \in \mathcal{V}\right\}$. Since the weight $\omega(p)$ of a walk $p=\left(v_{i}, v_{i}\right)$ in $\mathcal{L}(\mathcal{G})$ is equal to $d_{i}$, the first spectral moment is equal to:

$$
m_{1}\left(L_{\mathcal{G}}\right)=\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \omega\left(\left(v_{i}, v_{i}\right)\right)=\frac{1}{n} \sum_{i=1}^{n} d_{i}=\frac{1}{n} S_{1}
$$

In order to compute the second moment $m_{2}\left(L_{\mathcal{G}}\right)$, we need to account for two different types of closed walks of length two:
(a) Walks in $\mathcal{L}(\mathcal{G})$ of the first type visit a self-loop twice, i.e., $p=\left(v_{i}, v_{i}, v_{i}\right)$, and the weight of this walk is $d_{i}^{2}$. We denote the set containing walks of this type as $P_{2 a}^{(i)}$.
(b) Walks of the second type start at a node $v_{i}$, visit a neighbor $v_{j} \in \mathcal{N}_{i}$, and return to $v_{i}$. This type of walk defines
the set $P_{2 b}^{(i)} \triangleq\left\{\left(v_{i}, v_{j}, v_{i}\right)\right.$ for $\left.v_{i} \in \mathcal{V}, v_{j} \in \mathcal{N}_{i}\right\}$. The weight of any walk of this type is equal to 1 .

Since $P_{2 a}^{(i)} \cup P_{2 b}^{(i)}=P_{2, n}^{(i)}$ and $P_{2 a}^{(i)} \cap P_{2 b}^{(i)}=\emptyset$, the sets $P_{2 a}^{(i)}$ and $P_{2 b}^{(i)}$ form a partition of the set of walks $P_{2, n}^{(i)}$. Hence, from Lemma 3.1 we have

$$
\begin{aligned}
m_{2}\left(L_{\mathcal{G}}\right) & =\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{p \in P_{2 a}^{(i)}} \omega(p)+\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{p \in P_{2 b}^{(i)}} \omega(p) \\
& =\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} d_{i}^{2}+\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{v_{j} \in \mathcal{N}_{i}} 1 \\
& =\frac{1}{n} \sum_{i=1}^{n} d_{i}^{2}+\frac{1}{n} \sum_{i=1}^{n} d_{i}=\frac{1}{n}\left(S_{2}+S_{1}\right)
\end{aligned}
$$

In order to compute the third Laplacian spectral moment, we classify closed walks of length 3 in $\mathcal{L}(\mathcal{G})$ into sets that partition $P_{3, n}^{(i)}$. In particular, we classify these closed walks with respect to the structure of the subgraph 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 3.2 , are isomorphi4 ${ }^{4}$. In Fig. 22 we depict the set of all possible nonisomorphic subgraphs covered by closed walks of length 3 (in solid lines). According to this classification, we have the following types of walks:
(a) Walks of the first type present the form $\left(v_{i}, v_{i}, v_{i}, v_{i}\right)$, covering the self-loop three times. The subgraph covered by this walk is the isolated node, represented in Fig. 22a). Although the walk covering this graph visits the self-loop $\left\{v_{i}, v_{i}\right\}$ (in dashed line in Fig. 2/a)), this self-loop is not part of the covered subgraph (according to Definition 3.2). The weights associated with walks of this type are equal to $d_{i}^{3}$, and we denote the set of this type of walks as $P_{3 a}^{(i)}$.
(b) Walks of the second type present the form $\left(v_{i}, v_{i}, v_{j}, v_{i}\right)$ and $\left(v_{i}, v_{j}, v_{j}, v_{i}\right)$ with $v_{j} \in \mathcal{N}_{i}$. The subgraph covered by these walks is the single edge in Fig. 2(b), where the selfloops (in dashed line) are used by the walks but not included in the subgraph. These two walks have weights $d_{i}$ and $d_{j}$, respectively, and are represented in Fig. 2b). We denote this set of walks as $P_{3 b}^{(i)}$.
(c) The last type of walk presents the form $\left(v_{i}, v_{j}, v_{k}, v_{i}\right)$ and $\left(v_{i}, v_{k}, v_{j}, v_{i}\right)$ for $v_{i} \sim v_{j} \sim v_{k} \sim v_{i}$. The subgraph covered by these walks is the triangle (Fig. 2 (c)). These walks have weights -1 and we denote this set of walks as $P_{3 c}^{(i)}$.

Since the sets $P_{3 a}^{(i)}, P_{3 b}^{(i)}$, and $P_{3 c}^{(i)}$ partition the set of closed walks $P_{3, n}^{(i)}$, we have that

$$
m_{3}\left(L_{\mathcal{G}}\right)=\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{x \in\{a, b, c\}} \sum_{p \in P_{3 x}^{(i)}} \omega(p) .
$$

We can now analyze each of the terms in the above summation. For convenience, we define $T_{3 x} \triangleq \frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{p \in P_{3 x}^{(i)}} \omega(p)$, and study each one of the terms $T_{3 x}$ for $x \in\{a, b, c\}$ :

[^4]
(a)

(b)

(c)

Fig. 2. Collection of possible subgraphs covered by closed walks of length 3. Since these subgraphs are simple, by definition, they do not contain self-loops (which are included in the figure for convenience in our derivations).
(a) For $x=a$, all the walks in $P_{3 a}^{(i)}$ have a weight equal to $d_{i}^{3}$. Hence, we have $T_{3 a}=\frac{1}{n} \sum_{i=1}^{n} d_{i}^{3}=S_{3} / n$.
(b) For $x=b$, the walks in $P_{3 b}^{(i)}$ have a weight equal to either $d_{i}$ or $d_{j}$. Then, we have:

$$
\begin{aligned}
T_{3 b} & =\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{v_{j} \in \mathcal{N}_{i}} d_{i}+\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{v_{j} \in \mathcal{N}_{i}} d_{j} \\
& =\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i j} d_{i}+\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i j} d_{j} \\
& =\frac{1}{n} \sum_{i=1}^{n} d_{i}^{2}+\frac{1}{n} \sum_{j=1}^{n} d_{j}^{2}=2 S_{2} / n
\end{aligned}
$$

(c) For $x=c$, we have $T_{3 c}=\frac{1}{n} \sum_{1 \leq i, j, k \leq n}(-1) t_{i j k}$, where $t_{i j k}$ is an indicator function that takes the value 1 when $v_{i} \sim v_{j} \sim v_{k} \sim v_{i}$ ( 0 , otherwise). Hence, $T_{3 c}=$ $\frac{6}{n} \sum_{1 \leq i<j<k \leq n}(-1) t_{i j k}$, where the coefficient 6 accounts for all the possible permutations of the three indexes $i, j$, and $k$. Hence, since $\sum_{1 \leq i<j<k \leq n} t_{i j k}=\Delta / n$ (where $\Delta$ is the total number of triangles), we have that $T_{3 c}=-6 \Delta / n$.

Finally, since $m_{3}\left(L_{\mathcal{G}}\right)=T_{3 a}+T_{3 b}+T_{3 c}$, we obtain the expression for the third moment in the statement of the theorem.

Remark 3.2: Theorem 3.2 relates purely algebraic properties - the spectral moments - to structural features of the network, namely the degree sequence and the number of triangles. The key concept behind the proof is the classification of closed walks into sets according the subgraph covered by these walks. This idea can be extended to higher-order moments, although the combinatorial analysis becomes more elaborate as we increase the order of the moments.

Remark 3.3: Notice that the power-sums of the degrees, $S_{p}$, and the number of triangles, $\Delta$, can be retrieved from the set of first-order neighborhoods, $\left\{\mathcal{G}_{i}^{(1)}\right.$ for all $\left.v_{i} \in \mathcal{V}\right\}$. Therefore, we can compute the first three Laplacian spectral moments from local structural measurements with radius 1. As we shall discuss below, it is possible to compute the first $2 r+1$ Laplacian spectral moments of a graph whenever we have access to the set of $r$-th order neighborhoods, $\left\{\mathcal{G}_{i}^{(r)}\right.$ for all $\left.v_{i} \in \mathcal{V}\right\}$.
2) Higher-Order Laplacian Spectral Moments: We now extend our analysis to 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:

$$
\begin{align*}
C_{d d} & \triangleq \frac{1}{n} \sum_{v_{i} \sim v_{j}} d_{i} d_{j}, \quad C_{d^{2} d} \triangleq \frac{1}{n} \sum_{v_{i} \sim v_{j}} d_{i}^{2} d_{j}  \tag{4}\\
C_{d t} & \triangleq \frac{1}{n} \sum_{v_{i} \in \mathcal{V}} d_{i} t_{i}, \quad C_{d^{2} t} \triangleq \frac{1}{n} \sum_{v_{i} \in \mathcal{V}} d_{i}^{2} t_{i} \\
C_{d q} & \triangleq \frac{1}{n} \sum_{v_{i} \in \mathcal{V}} d_{i} q_{i}, \quad D_{d d} \triangleq \frac{1}{n} \sum_{v_{i} \sim v_{j}} d_{i} d_{j}\left|\mathcal{N}_{i} \cap \mathcal{N}_{j}\right|
\end{align*}
$$

where $\left|\mathcal{N}_{i} \cap \mathcal{N}_{j}\right|$ is the number of common neighbors shared by $v_{i}$ and $v_{j}$. The above terms represent correlations between structural variables in the graph, some of which have already been studied extensively. For example, $C_{d d}$ and $C_{d^{2} d}$ are closely related to the widely studied assortativity coefficient [8], which measures the preference (or aversion) of nodes to attach to nodes presenting a similar degree. On the other hand, we find in (4) several correlation terms that have not been studied in such depth. For example, the terms $C_{d t}$ and $C_{d^{2} t}$ quantify the correlation between degrees and local clustering ${ }^{5}$ throughout the set of nodes. Although nontrivial variations of local clustering with respect to degrees have been reported in the complex networks literature [18], the effects in the network's behavior are not well understood.

The main result in this section relates the fourth and fifth Laplacian spectral moments to local structural measurements and correlation terms, as follows:

Theorem 3.3: Let $\mathcal{G}$ be a simple graph with Laplacian matrix $L_{\mathcal{G}}$. Then, the fourth and fifth Laplacian moments can be written as

$$
\begin{align*}
m_{4}\left(L_{\mathcal{G}}\right)= & \frac{1}{n}\left(-S_{1}+2 S_{2}+4 S_{3}+S_{4}+8 Q\right)  \tag{5}\\
& +4 C_{d d}-8 C_{d t} \\
m_{5}\left(L_{\mathcal{G}}\right)= & \frac{1}{n}\left(-5 S_{2}+5 S_{3}+5 S_{4}+S_{5}+30 \Delta-10 P\right) \\
& +10\left(C_{d d}+C_{d^{2} d}-C_{d t}-C_{d^{2} t}+C_{d q}-D_{d d}\right)
\end{align*}
$$

where $S_{p}$ is defined in (1), and the correlation terms $C_{d d}, C_{d t}$, $C_{d q}, C_{d^{2} d}, C_{d^{2} t}$, and $D_{d d}$ are defined in (4).

Proof: As in Theorem 3.2, the proof is based on a classification of closed walks of length 4 and 5 with respect to the subgraph covered by the walks. Details about this classification and the subsequent combinatorial analysis can be found in the Appendix.

Remark 3.4: Observe how, as we increase the order of the moments, more complicated structural features arise in our expressions. In particular, the fifth moment is influenced by the degree sequence, the number of cycles of length 3 and 5, and all the correlation terms defined in (4).

Remark 3.5: As we mentioned before, the maximum order of the spectral moment that one can compute from local structural information depends on the radius $r$ of the neighborhoods that are accessible to us. One can prove that in order to compute the $k$-th Laplacian spectral moment, we need to count

[^5]the number of cycles of length $k$ in $\mathcal{G}$. One can also prove that access to neighborhoods of radius $r$ allows us to count all cycles of length up to $2 r+1$ in $\mathcal{G},[19]$. Hence, we can compute the set of Laplacian moments up to the order $k_{\max }=2 r+1$ using local structural information that can be extracted from the set of $r$-th order neighborhoods, $\left\{\mathcal{G}_{i}^{(r)}\right.$ for all $\left.v_{i} \in \mathcal{V}\right\}$.

In this section, we have derived expressions to compute the first five spectral moment of the Laplacian matrix of a network from local structural measurements. 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.

## IV. 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 $\left(m_{i}\left(L_{\mathcal{G}}\right)\right)_{i=1}^{k}$, find bounds on the spectral gap and the spectral radius of the Laplacian matrix $L_{\mathcal{G}}$.

Our results are based on an optimization framework recently proposed in [20]. In order to adapt our problem to this framework, we need to introduce some definitions. Given a simple connected graph $\mathcal{G}$ with Laplacian eigenvalues $\left\{\lambda_{i}\right\}_{i=1}^{n}$, we define the spectral density of the nontrivial eigenvalue spectrum as

$$
\begin{equation*}
\rho_{\mathcal{G}}(\lambda) \triangleq \frac{1}{n-1} \sum_{i \geq 2} \delta\left(\lambda-\lambda_{i}\right) \tag{6}
\end{equation*}
$$

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 ${ }^{6}$ of $\rho_{\mathcal{G}}(\lambda)$ is equal to $\operatorname{supp}\left(\rho_{\mathcal{G}}\right)=$ $\left\{\lambda_{i}\right\}_{i=2}^{n}$. The moments of the spectral density in 6p, denoted by $\bar{m}_{k}\left(L_{\mathcal{G}}\right)$, can be written in terms of the spectral moments of $L_{\mathcal{G}}$, as follows

$$
\begin{align*}
\bar{m}_{k}\left(L_{\mathcal{G}}\right) & \triangleq \int_{\mathbb{R}} \lambda^{k} \frac{1}{n-1} \sum_{i=2}^{n} \delta\left(\lambda-\lambda_{i}\right) d \lambda \\
& =\frac{1}{n-1} \sum_{i=2}^{n} \lambda_{i}^{k}=\frac{n}{n-1} m_{k}\left(L_{\mathcal{G}}\right) \tag{7}
\end{align*}
$$

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 [20]. In that paper, the following problem was addressed:

Problem 2: Consider a truncated sequence of moments $\left(M_{r}\right)_{1 \leq r \leq k}$ corresponding to an unknown density function $\mu(\lambda)$. Denote by $[a, b]$ the smallest interval containing the

[^6]support of $\mu$. 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 our spectral problem, we have a truncated sequence of five spectral moments, $\left(m_{r}\left(L_{\mathcal{G}}\right)\right)_{1 \leq r \leq 5}$, corresponding to the unknown density function $\rho_{\mathcal{G}}$ and given by the expressions (3), (5), and (7). In this context, the smallest interval $[a, b]$ containing $\operatorname{supp}\left(\rho_{\mathcal{G}}\right)$ is equal to $\left[\lambda_{2}, \lambda_{n}\right]$. 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 by Lasserre in [20] 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 $\mathbf{M}=\left(M_{r}\right)_{r=1}^{2 s+1}$, associated with an unknown density function $\mu$. We define the following Hankel matrices of moments:

$$
\begin{gather*}
R_{2 s}(\mathbf{M}) \triangleq\left[\begin{array}{cccc}
1 & M_{1} & \cdots & M_{s} \\
M_{1} & M_{2} & \cdots & M_{s+1} \\
\vdots & \vdots & \ddots & \vdots \\
M_{s} & M_{s+1} & \cdots & M_{2 s}
\end{array}\right],  \tag{8}\\
R_{2 s+1}(\mathbf{M}) \triangleq\left[\begin{array}{cccc}
M_{1} & M_{2} & \cdots & M_{s+1} \\
M_{2} & M_{3} & \cdots & M_{s+2} \\
\vdots & \vdots & \ddots & \vdots \\
M_{s+1} & M_{s+2} & \cdots & M_{2 s+1}
\end{array}\right] . \tag{9}
\end{gather*}
$$

We also define the localizing matrix $\left.{ }^{7}\right] H_{s}(x, \mathbf{M})$ as,

$$
\begin{equation*}
H_{s}(x, \mathbf{M}) \triangleq R_{2 s+1}(\mathbf{M})-x R_{2 s}(\mathbf{M}) \tag{10}
\end{equation*}
$$

The localizing matrix presents the following two properties [21]:

P1. $\quad H_{s}(\alpha, \mathbf{M}) \succeq 0$, if the support of $\mu$ is contained in the set $[\alpha, \infty)$, and
P2. $-H_{s}(\beta, \mathbf{M}) \succeq 0$, if the support of $\mu$ is contained in the set $(-\infty, \beta]$.
Based on these properties, Lasserre proposed the following series of SDP's to find a solution for Problem 2.

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

$$
\begin{align*}
& a \leq \alpha_{s}(\mathbf{M}) \triangleq \max _{x}\left\{x: H_{s}(x, \mathbf{M}) \succeq 0\right\}  \tag{11}\\
& b \geq \beta_{s}(\mathbf{M}) \triangleq \min _{x}\left\{x:-H_{s}(x, \mathbf{M}) \succeq 0\right\} \tag{12}
\end{align*}
$$

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

Remark 4.1: Note that the entries of the localizing matrix $H_{s}(x, \mathbf{M})$ depend affinely on the decision variable $x$. Thus, $\alpha_{s}(\mathbf{M})$ and $\beta_{s}(\mathbf{M})$ are the solutions to two SDP's in one variable, which can be efficiently solved using standard optimization software.

[^7]Therefore, we can directly apply the above result to solve Problem 1 by considering the sequence of moments $\overline{\mathbf{m}} \triangleq$ $\left(\bar{m}_{r}\left(L_{\mathcal{G}}\right)\right)_{r=1}^{2 s+1}=\left(\frac{n}{n-1} m_{r}\left(L_{\mathcal{G}}\right)\right)_{r=1}^{2 s+1}$ in the statement of the solution to Problem 2 . Since this sequence of moments corresponds to the spectral density $\rho_{\mathcal{G}}$, with support $\left\{\lambda_{i}\right\}_{i=2}^{n}$, the solutions in (11) and (12) directly provide the following bounds on the spectral radius and spectral gap:

Solution to Problem 1 : Let $\overline{\mathbf{m}} \triangleq\left(\frac{n}{n-1} m_{r}\left(L_{\mathcal{G}}\right)\right)_{r=1}^{2 s+1}$ 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:

$$
\begin{align*}
& \lambda_{2} \leq \alpha_{s}(\overline{\mathbf{m}}) \triangleq \max _{x}\left\{x: H_{s}(x, \overline{\mathbf{m}}) \succeq 0\right\}  \tag{13}\\
& \lambda_{n} \geq \beta_{s}(\overline{\mathbf{m}}) \triangleq \min _{x}\left\{x:-H_{s}(x, \overline{\mathbf{m}}) \succeq 0\right\} \tag{14}
\end{align*}
$$

In Section III-B, we derived expressions for the first five Laplacian spectral moments, $\left(m_{r}\left(L_{\mathcal{G}}\right)\right)_{r=1}^{5}$, in terms of local structural measurements of the network. Therefore, we can apply the above solution to find spectral bounds for $s=2$. Furthermore, for $s=2$ we can prove that the optimal values $\alpha_{2}(\overline{\mathbf{m}})$ and $\beta_{2}(\overline{\mathbf{m}})$ are the maximum and minimum roots of a cubic polynomial, as follows. For $s=2$, the localizing matrix ${ }^{8}$ takes the form

$$
H_{2}(x, \overline{\mathbf{m}})=\left[\begin{array}{ccc}
\bar{m}_{1}-x & \bar{m}_{2}-x \bar{m}_{1} & \bar{m}_{3}-x \bar{m}_{2} \\
\bar{m}_{2}-x \bar{m}_{1} & \bar{m}_{3}-x \bar{m}_{2} & \bar{m}_{4}-x \bar{m}_{3} \\
\bar{m}_{3}-x \bar{m}_{2} & \bar{m}_{4}-x \bar{m}_{3} & \bar{m}_{5}-x \bar{m}_{4}
\end{array}\right] .
$$

Let us first analyze the optimal value $\beta_{2}(\overline{\mathbf{m}})$ in 14. Note that $-H_{2}(x, \overline{\mathbf{m}}) \succeq 0$ if and only if all the eigenvalues of $H_{2}(x, \overline{\mathbf{m}})$ are nonpositive. The characteristic polynomial of $H_{2}(x, \overline{\mathbf{m}})$ can be written as,

$$
\begin{aligned}
\phi_{2}(\lambda) & \triangleq \operatorname{det}\left(\lambda I-H_{2}(x, \overline{\mathbf{m}})\right) \\
& =\lambda^{3}+r_{1}(x) \lambda^{2}+r_{2}(x) \lambda+r_{3}(x)
\end{aligned}
$$

where $r_{j}(x)$ is a polynomial of degree $j$ in the variable $x$ (with coefficients depending on the sequence of moments $\left.\left(\bar{m}_{1}, \ldots, \bar{m}_{5}\right)\right)$. One can prove that all the eigenvalues of the Hankel matrix $H_{2}(x, \overline{\mathbf{m}})$ are real [22]. Also, by Descartes' rule, all the roots of $\phi_{2}(\lambda)$ are nonpositive if and only if $r_{j}(x) \geq 0$, for $j=1,2$, and 3. Lasserre proved in [20] that $r_{j}(x) \geq 0$ if and only if $r_{3}(x) \geq 0$. Since $r_{3}(x)=$ $-\operatorname{det} H_{2}(x, \overline{\mathbf{m}})$, we have that the optimal value $\beta_{2}(\overline{\mathbf{m}})$ in (14) is equal to the largest root of the cubic polynomial $r_{3}(x)=-\operatorname{det} H_{2}(x, \overline{\mathbf{m}})=0$. Similarly, one can also prove that the optimal value $\alpha_{2}(\overline{\mathbf{m}})$ in 13) is the smallest root of $r_{3}(x)$. We now state this result more explicitly as follows:

Solution to Problem 1 with 5 Moments: Let $\overline{\mathbf{m}}=$ $\left(\frac{n}{n-1} m_{r}\left(L_{\mathcal{G}}\right)\right)_{r=1}^{5}$ 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

$$
\begin{align*}
& \lambda_{2} \leq \alpha_{2}(\overline{\mathbf{m}})=\min \left\{x_{1}, x_{2}, x_{3}\right\}  \tag{15}\\
& \lambda_{n} \geq \beta_{2}(\overline{\mathbf{m}})=\max \left\{x_{1}, x_{2}, x_{3}\right\}
\end{align*}
$$

where $x_{1}, x_{2}$, and $x_{3}$ are the roots of $r_{3}(x)=$ $-\operatorname{det} H_{2}(x, \overline{\mathbf{m}})$.

[^8]

Fig. 3. In (a), we plot the complementary cumulative distribution of degrees for the electrical transmission network under study. In (b), we plot the joint-degree distribution $J_{d}\left(k_{1}, k_{2}\right)$ in the range $1 \leq k_{1}, k_{2} \leq 9$ for the American power grid. In (c), we plot on a semilogarithmic scale the number of cycles $\phi_{l}$ in the three transmission networks for lengths $3 \leq l \leq 10$.

Remark 4.2: Note that it is easy, but tedious, to write down an explicit expression for $r_{3}(x)$ in terms of the Laplacian spectral moments. Also, we can find explicit expressions for the roots of the cubic polynomial $r_{3}(x)$ using, for example, Cardano's rule [23]. Therefore, it is possible to derive explicit expressions for $\alpha_{2}(\overline{\mathbf{m}})$ and $\beta_{2}(\overline{\mathbf{m}})$ in terms of the Laplacian spectral moments, but the resulting expressions are so complicated that they do not provide much insight.

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. These spectral moments can be written in terms of local structural measurements using (3) and (5). Hence, our results build a bridge between structural measurements of a network and its spectral properties. In the following section, we use our theoretical results to analyze spectral properties of electrical transmission networks.

## V. Structural Analysis and Simulations

Motivated by recent interest for smart grid architectures, there is a fast-growing literature studying the structure and function of electrical transmission and distribution networks [24]-[26]. Most of the results found in the literature make use of extensive numerical simulations to find relationships between structural properties of a power grid and the behavior of dynamical processes taking place within it. In this section, we apply our theoretical results to study the relationship between structural and spectral properties of the American (western states), French and Spanish transmission networks. Our analysis reveals that the Laplacian spectral radii and spectral moments of electrical transmission networks are strongly constrained by the degree sequence and the so-called jointdegree distribution. We also verify that the spectral gap cannot be efficiently bounded using local structural features only, since this spectral property strongly depends on the global connectivity of the network.

## A. Local Structural Analysis

We examine unweighted, undirected graphs representing the structure of high-voltage transmission networks in the USA
(western states), France and Spain (the adjacencies of these networks are available, in MATLAB format, in [27]). The number of nodes (buses) and edges (transmission lines) in these networks are: $n_{u s}=4,941$ and $e_{u s}=6,594$ for the American network, $n_{f r}=146$ and $e_{f r}=223$ for the French, and $n_{s p}=98$ and $e_{s p}=175$ for the Spanish. From these data sets, we compute a collection of structural features that are relevant to the network's functionality.

We begin our structural analysis by studying the distribution of degrees in the network. In the network science literature, it is common to classify the degree distribution by looking at the complementary cumulative distribution function (CCDF) of the degrees, denoted by $\operatorname{ccdf}(k)$. The function $\operatorname{ccdf}(k)$ is defined as the probability that a node chosen uniformly at random presents a degree higher than or equal to a given value $k$. In Fig. 3(a) we plot the CCDF's for the three transmission networks under study. These distributions are well approximated by exponential functions [24].

Another extensively studied structural property is the jointdegree distribution. This distribution is related to the number of edges connecting sets of nodes of different degrees [28], and it is defined as follows: Consider the sets of nodes with degrees $k_{1}$ and $k_{2}$, denoted by $\mathcal{V}_{k_{1}}$ and $\mathcal{V}_{k_{2}}$; then, the jointdegree distribution is defined as:

$$
J_{d}\left(k_{1}, k_{2}\right) \triangleq \frac{1}{2 e} \sum_{v_{i} \in \mathcal{V}_{k_{1}}} \sum_{v_{j} \in \mathcal{V}_{k_{2}}} a_{i j}
$$

where $e$ is the total number of edges in the network. The correlation terms $C_{d d}$ and $C_{d^{2} d}$ defined in (4) can be explicitly related to the joint-degree distribution, as follows

$$
\begin{aligned}
C_{d d} & =\frac{e}{n} \sum_{k_{1}=1}^{d_{\max }} \sum_{k_{2}=1}^{d_{\max }} k_{1} k_{2} J_{d}\left(k_{1}, k_{2}\right) \\
C_{d^{2} d} & =\frac{e}{n} \sum_{k_{1}=1}^{d_{\max }} \sum_{k_{2}=1}^{d_{\max }} k_{1}^{2} k_{2} J_{d}\left(k_{1}, k_{2}\right)
\end{aligned}
$$

where $d_{\text {max }}$ is the network's maximum degree. In Fig. 3b), we plot a contour plot representing the joint-degree distribution of the American power grid (for $1 \leq k_{1}, k_{2} \leq 9$ ).

TABLE I
Summands involved in the first five Laplacian moments of the American grid.

| $k$ | $m_{k}$ | $\frac{\delta_{k}^{(1)} S_{1}}{n}$ | $\frac{\delta_{k}^{(2)} S_{2}}{n}$ | $\frac{\delta_{k}^{(3)} S_{3}}{n}$ | $\frac{\delta_{k}^{(4)} S_{4}}{n}$ | $\frac{\delta_{k}^{(5)} S_{5}}{n}$ | $\frac{\gamma_{k}^{(3)} \Delta}{n}$ | $\frac{\gamma_{k}^{(4)} Q}{n}$ | $\frac{\gamma_{k}^{(5)} P}{n}$ | $\eta_{k}^{(1)} C_{1}$ | $\eta_{k}^{(2)} C_{2}$ | $\eta_{k}^{(3)} C_{3}$ | $\eta_{k}^{(4)} C_{4}$ | $\eta_{k}^{(5)} C_{5}$ | $\eta_{k}^{(5)} C_{6}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 2.66 | $\mathbf{2 . 6 6}$ | - | - | - | - | - | - | - | - | - | - | - | - |  |
| 2 | 13.0 | $\mathbf{2 . 6 6}$ | $\mathbf{1 0 . 3 3}$ | - | - | - | - | - | - | - | - | - | - | - |  |
| 3 | 87.5 | - | $\mathbf{3 0 . 9 9}$ | $\mathbf{5 7 . 2 9}$ | - | - | -0.79 | - | - | - | - | - | - | - |  |
| 4 | 742.4 | -2.66 | 20.66 | $\mathbf{2 2 9 . 1}$ | $\mathbf{4 3 2 . 4}$ | - | - | 1.58 | - | $\mathbf{8 0 . 1 2}$ | - | - | -18.81 | - | - |
| 5 | 7,588 | - | -51.6 | 286.4 | $\mathbf{2 , 1 6 2}$ | $\mathbf{4 , 1 5 7}$ | 3.95 | - | -3.68 | 200.3 | $\mathbf{1}, \mathbf{1 2 7}$ | -23.51 | -177.2 | 5.30 | - |

A structural distribution that is relevant in our analysis is the number of cycles in the network (i.e., closed walks with no repeated nodes). We denote by $\phi_{l}$ the total number of cycles of length $l$ in the network, and plot $\phi_{l}$ versus $l$ for the three networks under consideration in Fig. 3(c).

In previous sections, we have provided tools that allow us to quantify the effects of these (and other) structural measurements on the Laplacian spectrum. We base our subsequent analysis on the closed-form expressions for the spectral moments in (3) and (5). Note that these expressions can be written in a unified form as follows:

$$
\begin{equation*}
m_{k}\left(L_{\mathcal{G}}\right)=\sum_{r=1}^{5} \delta_{k}^{(r)} \frac{S_{r}}{n}+\sum_{s=3}^{5} \gamma_{k}^{(s)} \frac{\phi_{s}}{n}+\sum_{t=1}^{6} \eta_{k}^{(t)} C_{t} \tag{16}
\end{equation*}
$$

where $S_{r}$ is the $r$-th power sum of the degrees, $\phi_{s}$ is the number of cycles of length $s$, and $C_{t}$ indicate the correlation terms with $\left(C_{t}\right)_{t=1}^{6}=\left(C_{d d}, C_{d^{2} d}, C_{d t}, C_{d^{2} t}, C_{d q}, D_{d d}\right)$. The coefficients $\delta_{k}^{(r)}, \gamma_{k}^{(s)}$, and $\eta_{k}^{(t)}$ are, respectively, the coefficients accompanying $S_{r} / n, \phi_{s} / n$, and $C_{t}$ in the expression for the $k$-th moment. For example, according to (3), the third spectral moment has coefficients $\delta_{3}^{(2)}=3, \delta_{3}^{(3)}=1$, and $\gamma_{3}^{(3)}=-6$ (and the rest of coefficients are zero).

We now use (16) to quantify the effect of relevant structural measurements on the spectral moments of the American power grid. In this network, the relevant structural measurements are: ( $i$ ) the power-sums of the degrees: $\left(S_{r}\right)_{r=1}^{5}=$ ( $2.669,10.33,57.29,432.4,4157$ ), (ii) the number of cycles: $\phi_{3}=\Delta=651, \phi_{4}=Q=979, \phi_{5}=P=1821$, and (iii) the correlation terms $C_{d d}=20.03, C_{d^{2} d}=112.7, C_{d t}=2.35$, $C_{d^{2} t}=17.72, C_{d q}=5.30$, and $D_{d d}=14.58$. In Table I. we include the values of each one of the summands in 16) for the first five Laplacian moments of the American power grid. In this table, we can detect those terms that dominate the sum for each spectral moment. We have marked (in bold numerals) those summands that individually account for over $10 \%$ of the total sum; the sum of these dominant terms in each case provides a very good approximation to $m_{k}$. We observe how the power-sums of the degree sequence $S_{r}$ have a large impact on all the spectral moments. Also, the correlation terms $C_{1}=C_{d d}$ and $C_{2}=C_{d^{2} d}$ are significantly important for the fourth and fifth moments.

From these empirical observations, we conclude that the degree sequence plays a key role in the Laplacian spectral moments, as expected. Furthermore, the correlation terms $C_{d d}$ and $C_{d^{2} d}$ also have an important influence on the spectral moments. Note that these correlation terms, defined in 44, directly depend on the joint-degree distribution, $J_{d}\left(k_{1}, k_{2}\right)$. We conclude that the structural measurements that are most relevant for the Laplacian eigenvalue spectrum are:
(i) The degree distribution, via the power-sums $S_{r}$.
(ii) The joint-degree distribution, via the correlation terms $C_{d d}$ and $C_{d^{2} d}$.

Other correlation terms and the distribution of cycles of lengths 3 to 5 have a weak influence on the spectral moments. Similar structural results are also observed for both the French and Spanish transmission networks. The methodology introduced here allows us to recognize the degree distribution and the joint-degree distribution as the structural properties that are most influential on the Laplacian spectraL moments of the electrical grids under study.

## B. Spectral Bounds from Structural Information

From the collection of structural measurements studied above, we compute the first five spectral moments for the transmission networks under study, seeTable II We then use these moments to compute bounds on the spectral gap and spectral radius, $\alpha_{2}$ and $\beta_{2}$, using the methodology described in Solution to Problem 1 with 5 Moments, in Section IV The numerical values for these bounds, as well as the exact values for the spectral gap and spectral radius, $\lambda_{2}$ and $\lambda_{n}$, are included in Table III In this table, we also include the values obtained for the bounds in [13] and [16] (which were described in Section III-A.

TABLE II
First five Laplacian moments.

|  | $m_{1}\left(L_{G}\right)$ | $m_{2}\left(L_{G}\right)$ | $m_{3}\left(L_{G}\right)$ | $m_{4}\left(L_{G}\right)$ | $m_{5}\left(L_{G}\right)$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| USA | 2.66 | 13.00 | 87.50 | 742.4 | 7,588 |
| France | 3.05 | 15.58 | 97.73 | 680.1 | 5,046 |
| Spain | 3.57 | 20.83 | 147.3 | 1,155 | 9,686 |

TABLE III
UPPER AND LOWER BOUNDS ON THE LAPLACIAN SPECTRAL GAP AND SPECTRAL RADIUS, $\lambda_{2}$ AND $\lambda_{n}$.

| Network | $[13]$ | $\lambda_{2}\left(L_{G}\right)$ | $\alpha_{2}$ | $\beta_{2}$ | $\lambda_{n}\left(L_{G}\right)$ | $[16]$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| USA | $1.16 \mathrm{e}-4$ | $7.59 \mathrm{e}-4$ | 0.97 | 12.8 | 20.10 | 22.28 |
| France | $3.70 \mathrm{e}-3$ | $4.24 \mathrm{e}-2$ | 0.81 | 8.07 | 9.60 | 9.86 |
| Spain | $4.90 \mathrm{e}-3$ | $7.70 \mathrm{e}-2$ | 0.86 | 9.18 | 10.66 | 10.79 |

In Table III] we observe that $\beta_{2}$ and the bound in [16] strongly constrain the intervals of possible values for the spectral radii, specially in the case of European transmission networks. In Fig. 4(a)-(c), we plot the histograms for the Laplacian eigenvalues of the American (western states), French and Spanish transmission networks, where we have also included the bounds in Table III. We observe that bounds for the Laplacian spectral gap based on local structural measurements perform poorly in practice. The main reason


Fig. 4. In Figs. (a), (b) and (c), we plot histograms for the Laplacian eigenvalues of the American (western states), French and Spanish high-voltage transmission networks, respectively. In the small subfigures, we plot a histograms of the eigenvalues around the origin and indicate the spectral gap. We also include the values of the bounds of the Laplacian spectral radius and gap from Table III
behind this limitation is that the Laplacian spectral gap is a global property that quantifies how 'well-connected' a network is [29],[30]. 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.

## C. Spectrum-Preserving Structural Perturbations

In this subsection, we validate our previous structural analysis with numerical computations. One of our main conclusions is that the degree and joint-degree distributions are the structural features with the strongest influence on the Laplacian spectral moments and spectral radii of electrical transmission networks. We can empirically verify this conclusion by studying the effect of structural perturbations that preserve these features on the Laplacian spectrum. In what follows, we provide an algorithmic description of a structural perturbation that transforms an input graph $G_{i n}=\left(\mathcal{V}, \mathcal{E}_{i n}\right)$ into a different output graph $G_{\text {out }}=\left(\mathcal{V}, \mathcal{E}_{\text {out }}\right)$ while preserving both the degree and the joint-degree distributions:
(i) Randomly choose two degrees $k_{1}$ and $k_{2}$ drawn from the joint-degree probability distribution $J_{d}\left(k_{1}, k_{2}\right)$.
(ii) Choose two edges $\left\{v_{i}, v_{j}\right\}$ and $\left\{v_{r}, v_{s}\right\}$ uniformly at random from the set of edges in $\mathcal{E}_{i n}$ that satisfy $d_{i}=d_{r}=k_{1}$ and $d_{j}=d_{s}=k_{2}$.
(iii) Build an intermediate network $F=\left(\mathcal{V}, \mathcal{E}^{+}\right)$, where

$$
\mathcal{E}^{+} \triangleq \mathcal{E}_{i n}+\left\{v_{i}, v_{s}\right\}+\left\{v_{r}, v_{j}\right\}-\left\{v_{i}, v_{j}\right\}-\left\{v_{r}, v_{s}\right\}
$$

i.e., remove edges $\left\{v_{i}, v_{j}\right\}$ and $\left\{v_{r}, v_{s}\right\}$, and add edges $\left\{v_{i}, v_{s}\right\}$ and $\left\{v_{r}, v_{j}\right\}$.
(iv) If $F$ is connected and has no multi-edges (several edges connecting the same pair of nodes), we define the output rewired network $G_{\text {out }} \triangleq F$. Else, go to step (i).

Note that the above algorithm defines a random rewiring that maintains both the degree distribution and the jointdegree distribution of $G_{i n}$, since the number edges between the sets of nodes with degrees $k_{1}$ and $k_{2}$, denoted by $\mathcal{V}_{k_{1}}$ and $\mathcal{V}_{k_{2}}$, is not modified. Since these structural properties have the strongest influence on the Laplacian spectral moments, we should expect the Laplacian spectrum to remain almost invariant. In order to verify this statement, we recursively apply this random rewiring 5,000 times to the American
power grid. We can verify that, despite the large number of rewirings, the spectral radii and spectral moments of the resulting network, which we denote by $\mathcal{G}_{r w}$, are practically identical to those of the American power grid. In particular, the percentage of change in the first five spectral moments of $\mathcal{G}_{r w}$ is under $0.5 \%$. Furthermore, the spectral radius of $\mathcal{G}_{r w}$ is 20.18 , which represents a $0.36 \%$ change with respect to the original network. As expected, the spectral property that is most sensitive to the rewirings is the spectral gap, which takes a resulting value of 0.016 (from a value of $\lambda_{2}=8.4 e-4$ for the American grid).

## VI. Conclusions

This paper studies the relationship between local structural features of large complex networks and global spectral properties of their Laplacian matrices. We have proposed a novel approach, based on algebraic graph theory and convex optimization, that allows us to quantify the effect of an important collection of local structural features on the Laplacian spectral moments and spectral radius. The following is a list of our main contributions and conclusions:

1) We have derived in Section III-B explicit expressions to compute the first $2 k+1$ spectral moments of the Laplacian matrix using local structural measurements with radius $r$.
2) We have proposed an optimization framework in Section IV to compute lower bounds on the spectral radius of the Laplacian matrix 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 structural correlations.
3) Our analysis reveals that the local structural measurements that are most relevant to the Laplacian spectrum of electrical transmission networks are the degree sequence and joint-degree distributions. We have numerically verified that other structural properties that may seem important, such as the distribution of short cycles in the network, have a very weak influence on the Laplacian spectrum.
4) As expected, local structural features are not enough to efficiently bound or estimate the Laplacian spectral gap, since this spectral property strongly depends on the global connectivity of the network. Since the spectral gap is fundamental in the analysis of many dynamical processes on networks, random models in which only local structural features are prescribed, such as those in [7]-[9], are not valid to generate synthetic topologies in which these dynamical processes can be studied.
Although the mathematical tools developed here can be extended to the case of weighted networks, we have limited our analysis to unweighted networks to isolate the role played by the network topological structure from other factors. Ongoing work addresses the spectral analysis of large-scale networks with weighted edges, as well as networks with directed edges.

Finally, the analytical approach introduced is also applicable to the analysis of spectral properties of many real networks in other areas of science and technology, such as networks of multi-agent systems, communication networks, as well as social and biological networks. Since the Laplacian eigenvalues are relevant in a wide variety of dynamical processes, our approach is useful to theoretically analyze the effect of local structural properties on those processes.

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## Appendix

Theorem 3.3 Let $\mathcal{G}$ be a simple graph with Laplacian matrix $L_{\mathcal{G}}$. Then, the fourth and fifth Laplacian moments can be written as

$$
\begin{aligned}
m_{4}\left(L_{\mathcal{G}}\right)= & \frac{1}{n}\left(-S_{1}+2 S_{2}+4 S_{3}+S_{4}+8 Q\right) \\
& +4 C_{d d}-8 C_{d t}, \\
m_{5}\left(L_{\mathcal{G}}\right)= & \frac{1}{n}\left(-5 S_{2}+5 S_{3}+5 S_{4}+S_{5}+30 \Delta-10 P\right) \\
& +10\left(C_{d d}+C_{d^{2} d}-C_{d t}-C_{d^{2} t}+C_{d q}-D_{d d}\right)
\end{aligned}
$$

where $S_{r}=\sum_{v_{i} \in \mathcal{V}} d_{i}^{r}$, and the correlation terms $C_{d d}, C_{d t}$, $C_{d q}, C_{d^{2} d}, C_{d^{2} t}$, and $D_{d d}$ are defined in 4.

Proof: As in Theorem 3.2, we use Lemma 3.1 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. As we explained in the proof of Theorem 3.2, two walks of length 4 are in the same subset if the subgraphs they cover are isomorphic (without considering self-loops). We enumerate the possible types in Fig. 5 and we denote the corresponding sets of walks as $P_{4 a}^{(i)}, P_{4 b}^{(i)}, P_{4 c}^{(i)}, P_{4 d}^{(i)}$, and $P_{4 e}^{(i)}$. These sets $P_{4 a}^{(i)}, \ldots, P_{4 e}^{(i)}$ partition the set of closed walks $P_{4, n}^{(i)}$. Hence, we have

$$
m_{4}\left(L_{\mathcal{G}}\right)=\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{x \in\{a, b, c, d, e\}} \sum_{p \in P_{d x}^{(i)}} \omega(p) .
$$

We now analyze each one of the terms in the above summations. For convenience, we define $T_{4 x} \triangleq$

(a)

(b)

(c)

(d)

(e)

Fig. 5. Collection of possible graphs covered by closed walks of length 4.
$\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{p \in P_{4 x}^{(i)}} \omega(p)$ and analyze the term $T_{4 x}$ for $x \in$ $\{a, b, c, d\}$ :
(a) For $x=a$, we have that the weights $\omega(p)$ of the walks in $P_{4 a}^{(i)}$ are all the same, and equal to $d_{i}^{4}$. Hence

$$
T_{4 a}=\frac{1}{n} \sum_{i} d_{i}^{4}=S_{4} / n
$$

(b) For $x=b$, the weights of the walks in $P_{4 b}^{(i)}$ are equal to $2+4\left(d_{i}^{2}+d_{j}^{2}+d_{i} d_{j}\right)$. Hence

$$
\begin{aligned}
T_{4 b} & =\frac{1}{n} \sum_{v_{i} \sim v_{j}} 2+4\left(d_{i}^{2}+d_{j}^{2}+d_{i} d_{j}\right) \\
& =\frac{1}{n}\left(S_{1}+4 S_{3}\right)+4 C_{d d}
\end{aligned}
$$

(c) For $x=c$, the weights of the walks in $P_{4 c}^{(i)}$ (i.e., walks that cover the two-chain graph) are equal to 4 . Hence

$$
T_{4 c}=\frac{1}{n} \sum_{v_{j} \sim v_{i} \sim v_{k}} 4 \stackrel{(i)}{=} \frac{1}{n} \sum_{i=1}^{n}\binom{d_{i}}{2} 4=\frac{2}{n}\left(S_{2}-S_{1}\right)
$$

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 $P_{4 d}^{(i)}$ are equal to $-8\left(d_{i}+d_{j}+d_{k}\right)$. Hence,

$$
\begin{aligned}
T_{4 d} & =\frac{1}{n} \sum_{v_{i} \sim v_{j} \sim v_{k} \sim v_{i}}-8\left(d_{i}+d_{j}+d_{k}\right) \\
& =-\frac{8}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} 3 t_{i j k} d_{i}
\end{aligned}
$$

where $t_{i j k}$ is an indicator function that takes value 1 if $v_{i} \sim$ $v_{j} \sim v_{k} \sim v_{i}$. Since $\sum_{j=1}^{n} \sum_{k=1}^{n} 3 t_{i j k}=t_{i}$ (the number of triangles touching node $v_{i}$ ), we have that

$$
T_{4 d}=-\frac{8}{n} \sum_{i=1}^{n} t_{i} d_{i}=-8 C_{d t}
$$

(e) For $x=e$, the weights of the walks in $P_{4 e}^{(i)}$ are equal to 8. Hence,

$$
T_{4 e}=\frac{1}{n} \sum_{\substack{v_{i} \sim v_{j} \sim v_{k} \sim v_{r} \sim v_{i} \\ \text { s.t. } 1 \leq i<j<k<r \leq n}} 8=8 Q / n
$$

Finally, since $m_{4}\left(L_{\mathcal{G}}\right)=T_{4 a}+T_{4 b}+T_{4 c}+T_{4 d}$, 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. In this case, the algebraic manipulations become more tedious. Below, we provide the main steps in the derivations (and omit the details regarding the algebraic manipulations). 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. 6.

We now analyze each one of the terms $T_{5 x} \triangleq$ $\frac{1}{n} \sum_{v_{i} \in \mathcal{V}} \sum_{p \in P_{5 x}^{(i)}} \omega(p)$ for $x \in\{a, b, \ldots, g\}$ :
(a) For $x=a$, we have

$$
T_{5 a}=\frac{1}{n} \sum_{i=1}^{n} d_{i}^{5}=S_{5} / n
$$

(b) For $x=b$, we can determine all possible closed walks of length 5 using the edge graph in Fig. 6(b) and derive that

$$
\begin{aligned}
T_{5 b} & =\frac{1}{n} \sum_{v_{i} \sim v_{j}} 5\left(d_{i}+d_{j}+d_{i}^{3}+d_{j}^{3}+d_{i}^{2} d_{j}+d_{i} d_{j}^{2}\right) \\
& =\frac{5}{n}\left(S_{2}+S_{4}\right)+10 C_{d^{2} d}
\end{aligned}
$$

(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

$$
\begin{aligned}
T_{5 c} & =\frac{1}{n} \sum_{v_{j} \sim v_{i} \sim v_{k}} 10 d_{i}+5 d_{j}+5 d_{k} \\
& =\frac{10}{n} \sum_{i=1}^{n}\binom{d_{i}}{2} d_{i}+\frac{5}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i j}\left(d_{i}-1\right) d_{j}
\end{aligned}
$$

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 $\sum_{v_{j} \sim v_{i} \sim v_{k}} d_{j}=\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i j}\left(d_{i}-1\right) d_{j}$. Thus,
$T_{5 c}=\frac{5}{n} \sum_{i=1}^{n} d_{i}^{3}-\frac{5}{n} \sum_{i=1}^{n} d_{i}^{2}+\frac{5}{n} \sum_{1 \leq i, j \leq n} a_{i j} d_{i} d_{j}-\frac{5}{n} \sum_{j=1}^{n} d_{j}^{2}$
$=\frac{5}{n}\left(S_{3}-2 S_{2}\right)+10 C_{d d}$
(d) For $x=d$, we can determine all possible closed walks of length 5 using the edge graph in Fig. 6(d) and derive that

$$
\begin{aligned}
T_{5 d}= & \frac{1}{n} \sum_{v_{i} \sim v_{j} \sim v_{k} \sim v_{i}}-30-10\left(d_{i}^{2}+d_{j}^{2}+d_{k}^{2}\right. \\
& \left.+d_{i} d_{j}+d_{j} d_{k}+d_{k} d_{i}\right) \\
= & -\frac{30 \Delta}{n}-\frac{10}{n} \sum_{\substack{v_{i} \sim v_{j} \sim v_{k} \sim v_{i}}}\left(3 d_{i}^{2}+3 d_{i} d_{j}\right) \\
= & -\frac{30 \Delta}{n}-\frac{30}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} t_{i j k} d_{i}^{2} \\
& -\frac{5}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i j} b_{i j}\left(d_{i} d_{j}\right)
\end{aligned}
$$

where $b_{i j} \triangleq \sum_{k=1}^{n} a_{i k} a_{j k}=\left|\mathcal{N}_{i} \cap \mathcal{N}_{j}\right|$, the number of common neighbors shared by $v_{i}$ and $v_{j}$. Hence,

$$
\begin{aligned}
T_{5 d} & =-\frac{30 \Delta}{n}-\frac{10}{n} \sum_{i=1}^{n} t_{i} d_{i}^{2}-\frac{10}{n} \sum_{i \sim j} a_{i j} b_{i j}\left(d_{i} d_{j}\right) \\
& =-30 \Delta / n-10 C_{d^{2} t}-10 D_{d d}
\end{aligned}
$$

(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

$$
\begin{aligned}
T_{5 e} & =\frac{1}{n} \sum_{v_{i} \sim v_{j} \sim v_{k} \sim v_{r} \sim v_{i}} 10\left(d_{i}+d_{j}+d_{k}+d_{r}\right) \\
& =\frac{10}{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{r=1}^{n} 4 q_{i j k r} d_{i}
\end{aligned}
$$

where $q_{i j k r}$ is an indicator function that takes value 1 if $v_{i} \sim v_{j} \sim v_{k} \sim v_{r} \sim v_{i}$. Since $\sum_{1 \leq j, k, r \leq n} 4 q_{i j k r}=q_{i}$ (the number of quadrangles touching node $v_{i}$ ), we have that

$$
T_{5 e}=\frac{10}{n} \sum_{i=1}^{n} q_{i} d_{i}=10 C_{d q}
$$

(f) For $x=f$, we have 10 possible walks covering the subgraph in Fig. 6(f). Since each walks has a weight equal to -1 , we have that

$$
\begin{aligned}
T_{5 f} & =\frac{1}{n} \sum_{v_{i} \sim v_{j} \sim v_{k} \sim v_{i} \sim v_{r}}-10 \\
& =-\frac{10}{n} \sum_{i=1}^{n}\left(d_{i}-2\right) t_{i},
\end{aligned}
$$

where in the last equality we take into account that the number of subgraphs of the type depicted in Fig. 6(f) and centered at node $v_{i}$ is equal to the number of triangles touching node $v_{i}$, $t_{i}$, multiplied by $\left(d_{i}-2\right)$ (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

$$
\begin{aligned}
T_{5 f} & =-\frac{10}{n} \sum_{i=1}^{n} d_{i} t_{i}+\frac{10}{n} \sum_{i=1}^{n} 2 t_{i} \\
& =-10 C_{d t}+60 \Delta / n
\end{aligned}
$$

$(g)$ For $x=f$, we have 10 possible walks on the pentagon and the associated weight of each walk is -1 . Hence

$$
T_{5 g}=\frac{1}{n} \sum_{v_{i} \sim v_{j} \sim v_{k} \sim v_{r} \sim v_{s} \sim v_{i}}-10=-10 \mathrm{P} / n
$$

where $P$ is the total number of pentagons in $\mathcal{G}$.
Finally, since $m_{5}\left(L_{\mathcal{G}}\right)=T_{5 a}+T_{5 b}+\ldots+T_{5 g}$, we obtain the expression for the fifth Laplacian spectral moment in the statement of the theorem after simple algebraic simplifications.


Fig. 6. Collection of possible graphs covered by closed walks of length 5 .

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[^1]:    ${ }^{1}$ A self-loop is an edge of the type $\left\{v_{i}, v_{i}\right\}$.

[^2]:    ${ }^{2}$ The edge connectivity of a connected graph is the minimum number of edges whose removal renders a disconnected graph.

[^3]:    ${ }^{3}$ The complete loopy graph $J_{n}$ is the graph with node-set $\mathcal{V}=\left\{v_{1}, \ldots, v_{n}\right\}$ and edge-set $\mathcal{E}=\left\{\left\{v_{i}, v_{j}\right\}\right.$ for all $\left.v_{i}, v_{j} \in \mathcal{V}\right\}$.

[^4]:    ${ }^{4}$ Two graphs $G$ and $H$ are isomorphic if there is a bijection between the vertex sets $V(G)$ and $V(H), f: V(G) \rightarrow V(H)$, such that any two vertices $u$ and $v$ of $G$ are adjacenct in $G$ if and only if $f(u)$ and $f(v)$ are adjacent in $H$.

[^5]:    ${ }^{5}$ The local clustering coefficient is defined as $t_{i} /\binom{d_{i}}{2}$, [5].

[^6]:    ${ }^{6}$ Recall that the support of a density function $\mu$ on $\mathbb{R}$, denoted by $\operatorname{supp}(\mu)$, is the smallest closed set $B$ such that $\mu(\mathbb{R} \backslash B)=0$.

[^7]:    ${ }^{7}$ A more general definition of localizing matrix can be found in [21. For simplicity, we restrict our definition to the particular form used in our problem.

[^8]:    ${ }^{8}$ We shall remove the argument $L_{\mathcal{G}}$ from the Laplacian spectral moments $\bar{m}_{r}\left(L_{\mathcal{G}}\right)$, for simplicity in notation.

