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Some more interplay of the three Kirchhoffian indices

José Luis Palacios *

Electrical and Computer Engineering Department, The University of New Mexico, Albuquerque, NM 87131, USA

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ABSTRACT

For any simple connected undirected graph, and the random walk on it, we obtain a formula for the sum of all expected hitting times – normalized by the stationary distribution – expressed in terms of the eigenvalues of a certain *modified* Laplacian matrix. This allows us to find lower bounds for these sums of hitting times, as well as new lower bounds for the additive degree-Kirchhoff index, in terms of the multiplicative degree-Kirchhoff index and the Kirchhoff index, that improve other bounds found in the literature.

1. Introduction

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1, 2, \ldots, n\}$ and degrees d_i for $1 \le i \le n$, with δ and Δ the smallest and largest such degrees, respectively, and $d_G = \dfrac{2|E|}{n}$ the *average degree*. There is a family of resistive – or Kirchhoffian – descriptors $R^f(G)$, studied in Mathematical Chemistry, with the general formula

* Fax: +1 505 2778298.
E-mail address: jpalacios@unm.edu.

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$$R^f(G) = \sum_{i<j} f(i,j)R_{i,j}, \tag{1}$$

where R_{ij} is the effective resistance between vertices i and j and $f(i,j)$ is some real function of the vertices. Among these descriptors, the ones that have undergone a more intense scrutiny are the Kirchhoff index $R(G)$, the multiplicative degree-Kirchhoff index $R^*(G)$ and the additive degree-Kirchhoff index $R^+(G)$, defined by (1) when taking $f(i,j) = 1$, $f(i,j) = d_i d_j$ and $f(i,j) = d_i + d_j$, respectively, and introduced in [11,3,6] respectively.

A first observation concerning these indices is that their relationship is very clear when the graphs under consideration are trees. Indeed for any tree T, in the absence of cycles, the effective resistance between any two vertices coincides with the distance between those vertices, and the equalities found in [10] and [5], referred to the so-called Schultz and modified Schultz indices, become the following equalities for the Kirchhoffian indices:

$$R^+(T) = 4R(T) - n(n-1), \tag{2}$$

and

$$R^*(T) = 4R(T) - (2n-1)(n-1), \tag{3}$$

once the distances are replaced with the effective resistances in the original equations. Equalities such as (2) and (3) remain elusive for general graphs and instead a number of inequalities have been found for these resistive descriptors.

Another observation on the Kirchhoffian indices is that two of them have a simple expression in terms of certain eigenvalues, namely (see [7,22], and also [8] and [16] for alternative proofs)

$$R(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i}, \tag{4}$$

for $\lambda_1 \geq \ldots \geq \lambda_n = 0$ the eigenvalues of the Laplacian matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where $\mathbf{D}$ is the diagonal matrix with the degrees of the vertices in the diagonal, and $\mathbf{A}$ is the adjacency matrix of G. Likewise (see [3,15])

$$R^*(G) = 2|E| \sum_{i=2}^{n} \frac{1}{1-\alpha_i} = 2|E| \sum_{i=1}^{n-1} \frac{1}{\beta_i}, \tag{5}$$

for $1 = \alpha_1 > \alpha_2 \geq \ldots \geq \alpha_n \geq -1$ the eigenvalues of the transition probability matrix $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$ of the random walk on G, and for $2 \geq \beta_1 \geq \ldots \geq \beta_n = 0$ the eigenvalues of the normalized Laplacian matrix $\boldsymbol{\mathcal{L}} = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2}$.

These expressions for $R(G)$ and $R^*(G)$ have led to an abundant bibliography of bounds for these indices found by optimizing the summations in (4) and (5) in some way. See