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Upper and Lower Bounds for the Additive Degree–Kirchhoff Index

José Luis Palacios*

Departamento de Cómputo Científico y Estadística.
Universidad Simón Bolívar. Apartado 89,000. Caracas, Venezuela.

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Abstract

We give tight upper and lower bounds for the additive degree-Kirchhoff index of a connected undirected graph.

1 Introduction

The Kirchhoff index $R(G)$ of a connected undirected graph $G = (V, E)$ with vertex set $\{1, 2, \ldots, N\}$ and edge set E was defined by Klein and Randić [1] as

$$R(G) = \sum_{i<j} R_{ij} ,$$

where R_{ij} is the effective resistance of the edge ij. This index has undergone intense scrutiny in recent years and researchers have come up with several modifications to it that take into account the degrees of the graph under consideration. On the one hand, Chen and Zhang defined in [2] the degree-Kirchhoff index as

$$R^*(G) = \sum_{i<j} d_i d_j R_{ij} , \tag{1}$$

where d_i is the degree (i.e., the number of neighbors) of the vertex i. This index has been studied in [3–6]. On the other hand, Gutman et al. defined in [7] the degree resistance index as

$$R^+(G) = \sum_{i<j} (d_i + d_j) R_{ij}, \tag{2}$$

*E-mail: jopala@usb.ve

and worked on the identification of graphs with lowest such degree among unicyclic graphs. Perhaps it would be convenient to unify the nomenclature and call $R^*(G)$ the multiplicative degree-Kirchhoff index while calling $R^+(G)$ the additive degree-Kirchhoff index.

One fruitful viewpoint to this area is the probabilistic approach, that we have used in [3, 8–11], and can be summarized as follows: on the graph G we can define the simple random walk as the N-state Markov chain $X_n, n \geq 0$, with transition probability matrix $P = (p_{ij})$, $1 \leq i, j \leq N$, whose entries are zero unless i and j are neighbors, in which case it is given by

$$p_{ij} = \frac{1}{d_i} \ .$$

The stationary distribution π of this Markov chain, i.e., the unique left probabilistic eigenvector of P associated to the eigenvalue 1, is given by

$$\pi_i = \frac{d_i}{2|E|}, 1 \leq i \leq N, \tag{3}$$

where $|E|$ is the number of edges of G.

The hitting time T_b of the vertex b is the number of jumps that the walk takes until it lands on b, and its expected value when the walk starts at a is denoted by E_aT_b. It is well known (see [8])that

$$R_{ij} = \frac{1}{2|E|}(E_iT_j + E_jT_i). \tag{4}$$

The purpose of this article is to give bounds for the additive degree-Kirchhoff index. On the one hand, we give a simple upper bound that is shown to be attained, except for the constant of the largest term, by the symmetric barbell graph. On the other hand, we use probabilistic arguments in order to get a general formula for $R^+(G)$ in terms of Kemeny's constant and a sum of hitting times normalized by the stationary distribution, that have lower bounds known in the Markov chain literature; this way we obtain a lower bound for $R^+(G)$ that is attained by the complete graph.

2 The bounds

For the upper bound, it is immediate that

$$R^+(G) \leq 2(N-1)R(G) \leq \frac{1}{3}(N^4 - N^3 - N^2 + N),$$

using the upper bound for $R(G)$, which occurs in the linear graph, obtained in [8]. The linear graph, however, with an additive degree-Kirchhoff index of order N^3 only, is a poor maximal candidate. We look instead at the $(aN, bN, (1-a-b)N)$ barbell graph, where $0 \leq a, b$; $a+b \leq 1$, which consists of two complete graphs on aN and bN vertices united by a path of length $(1-a-b)N$ (we allow ourselves some leeway regarding whether aN, bN and $(1-a-b)N$ are integers) and will show that the index is maximized when $a = b = \frac{1}{3}$.

Indeed, every pair of vertices, each of which belongs to a complete part, contributes roughly

$$(a+b)(1-a-b)N^2$$

to the sum (2). Since there are roughly abN^2 such pairs, the net contribution to the coefficient of N^4 of these vertices is

$$ab(a+b)(1-a-b). \tag{5}$$

Also, each vertex in the aN-complete part contributes, when adding the contributions of all vertices in the linear part, about $aN(1-a-b)^2N^2/2$. Taking into account all aN vertices in the aN complete part we obtain $a^2(1-a-b)^2/2N^4$. Repeating the argument with the bN part and adding to (5), and given that all other contributions generate lower powers of N, we find that the coefficient of N^4 is given by

$$ab(a+b)(1-a-b) + (a^2+b^2)(1-a-b)^2/2 =$$

$$a^2 + b^2 - 2a^3 - 2b^3 + a^4 + b^4 - 2a^2b^2. \tag{6}$$

Partial differentiation of the bivariate function $F(a,b)$ given by (6) shows that its critical points are $(0,0)$ (corresponding to the linear graph, without N^4 term), $(0,1),(1,0)$ (the complete graph, again, without N^4 term), $(0,\frac{1}{2}),(\frac{1}{2},0)$ (the lollipop graph, for which $R^+(G) \sim \frac{1}{16}N^4$) and $(\frac{1}{3},\frac{1}{3})$, (the symmetric $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ barbell graph, where the maximum is attained, with value $R^+(G) \sim \frac{2}{27}N^4$). We conjecture that this maximal value among all barbell graphs is indeed the maximum over all graphs on N vertices.

Now we work on the lower bound. From (2), (3) and (4), it is clear that

$$R^+(G) = \sum_{i<j}(\pi_i + \pi_j)(E_iT_j + E_jT_i)$$

$$= \sum_{i=1}^{N}\sum_{j\neq i}\pi_j E_iT_j + \sum_{j=1}^{N}\sum_{i\neq j}\pi_i E_iT_j.$$

It is well known (see [3, 12]) that the sum $\sum_j \pi_j E_i T_j$ is a constant K independent of i, usually called Kemeny's constant, that can be expressed in terms of the eigenvalues $\lambda_i \neq \lambda_1 = 1$ of the matrix P as

$$K = \sum_{i=2}^{N} \frac{1}{1-\lambda_i}.$$

It is also known (see [3]) that the multiplicative degree-Kirchhoff index can be written as

$$R^*(G) = 2|E|K.$$

Therefore

$$R^+(G) = NK + \sum_{j=1}^{N} \sum_{i \neq j} \pi_i E_i T_j = \frac{N}{2|E|} R^*(G) + \sum_{j=1}^{N} \sum_{i \neq j} \pi_i E_i T_j, \tag{7}$$

showing a relationship between the two degree-Kirchhoff indices.

The sum $\sum_i \pi_i E_i T_j$ in general depends on j, but there is a well known lower bound (see [12]) stating that

$$\sum_i \pi_i E_i T_j \geq \frac{1}{\pi_j}(1-\pi_j)^2.$$

Inserting this into (7) we obtain

$$R^+(G) \geq NK + \sum_{j=1}^{N} \frac{1}{\pi_j}(1-\pi_j)^2 = NK + \sum_{j=1}^{N} \frac{1}{\pi_j} - 2N + 1$$

$$= N \sum_{i=2}^{N} \frac{1}{1-\lambda_i} + 2|E| \sum_{j=1}^{N} \frac{1}{d_j} - 2N + 1. \tag{8}$$

Two applications of the harmonic mean-arithmetic mean inequality to equation (8), and the facts that $\sum_{i=2}^{N} \lambda_i = -1$ and $\sum_{j=1}^{N} d_j = 2|E|$, allow us to conclude that

$$R^+(G) \geq 2(N-1)^2,$$

a bound that is attained by the complete graph K_N, as an easy computation shows.

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