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Bounds for the Kirchhoff index via majorization techniques

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Abstract Using a majorization technique that identifies the maximal and minimal vectors of a variety of subsets of $\mathbb{R}^n$, we find upper and lower bounds for the Kirchhoff index $K(G)$ of an arbitrary simple connected graph G that improve those existing in the literature. Specifically we show that

$$K(G) \geq \frac{n}{d_1}\left[\frac{1}{1+\frac{\sigma}{\sqrt{n-1}}} + \frac{(n-2)^2}{n-1-\frac{\sigma}{\sqrt{n-1}}}\right],$$

where d_1 is the largest degree among all vertices in G,

$$\sigma^2 = \frac{2}{n}\sum_{(i,j)\in E}\frac{1}{d_i d_j} = \left(\frac{2}{n}\right) R_{-1}(G),$$

and $R_{-1}(G)$ is the general Randić index of G for $\alpha = -1$. Also we show that

$$K(G) \leq \frac{n}{d_n}\left(\frac{n-k-2}{1-\lambda_2} + \frac{k}{2} + \frac{1}{\theta}\right),$$

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where d_n is the smallest degree, λ_2 is the second eigenvalue of the transition probability of the random walk on G,

$$k = \left\lfloor \frac{\lambda_2 (n-1) + 1}{\lambda_2 + 1} \right\rfloor \quad \text{and} \quad \theta = \lambda_2 (n-k-2) - k + 2.$$

Keywords Majorization · Schur-convex functions · Graphs · Kirchhoff index

1 Introduction

The *Kirchhoff index* $K(G)$ of a simple connected graph $G = (V, E)$ with vertex set $V = \{1, 2, \ldots, n\}$ and edge set E was defined by Klein and Randić in [12] as

$$K(G) = \sum_{i<j} R_{ij}, \tag{1}$$

where R_{ij} is the effective resistance between vertices i and j, which can be computed using Ohm's law. This index has undergone intense scrutiny in recent years in the Mathematical Chemistry milieu because it has proven to be useful in discriminating among chemical molecules according to their cyclicity. A variety of techniques have been used, including graph theory, algebra (the study of the Laplacian and of the normalized Laplacian), electric networks, probabilistic arguments involving hitting times of random walks, and discrete potential theory (equilibrium measures and Wiener capacities), among others. The references that follow are a sample, by no means exhaustive, of these diverse techniques, whose end results usually follow either of these two paths: on the one hand, exact values for $K(G)$ are obtained for graphs endowed with some form of symmetry or special property [1,7,17,28]; on the other hand, general bounds for $K(G)$ are found in terms of invariants of G such as $|V|$, $|E|$, etc., and sometimes extremal graphs are found for specific families of graphs, as in [18,25,29] and [30].

In what follows we adopt this latter approach of finding upper and lower bounds for $K(G)$, with a technique from real analysis, namely majorization order and Schur-convexity, that adds new insights and is flexible enough to produce improvements of known bounds.

Schur-convexity and majorization order are widely discussed in [16]. It is worth pointing out previous uses of the majorization partial order in chemistry and a general overview is given in Klein [11]. Indeed, the degree-sequence partial order has previously been studied from a chemical perspective in [23,13]. By the property that Schur-convex functions preserve the majorization order, useful characterizations of extremal vectors of suitable subsets of $\mathbb{R}^n$ can be derived. Significant applications of this methodology concern the localization of real spectrum matrices [2,24]. More recently the problem of determining bounds for some relevant topological indicators of graphs which can be usefully expressed as Schur-convex functions has been investigated in [3,4] and [8]. One major advantage of this technique is to provide a unified approach to recover many bounds in the literature as well as to obtain better ones.

In this paper, after some preliminary definitions and notations concerning basic graph theory and the majorization order, we recall some results given in [3] aimed to determine extremal vectors with respect to majorization order of suitable subsets of $\mathbb{R}^n$. In Sect. 3, we adopt this technique to provide new upper and lower bounds for the Kirchhoff index both of general graphs and of particular classes of graphs. Next, some theoretical and numerical examples are presented, comparing our results with the literature. We conclude with some remarks regarding the degree-Kirchhoff index, another index loosely related to the Kirchhoff index.

2 Notations and preliminaries

Let us recall some basic graph notations (for more details we refer to [9] and [26]).

Let $G = (V, E)$ be a simple, connected, undirected graph where $V = \{1, 2, \dots, n\}$ is the set of vertices and $E \subseteq V \times V$ the set of edges, $|E| = m$.

The degree sequence of G is denoted by $\pi = (d_1, d_2, \dots, d_n)$ and it is arranged in non- increasing order $d_1 \geq d_2 \geq \cdots \geq d_n$, where d_i is the degree of vertex i. The equality $\sum_{i=1}^{n} d_i = 2m$ holds.

Let A be the adjacency matrix of G and $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$ be the set of its (real) eigenvalues. Given the diagonal matrix D of vertex degrees, the matrix $L = D - A$ is known as the Laplacian matrix of G. Let $\lambda_1(L) \geq \lambda_2(L) \geq \cdots \geq \lambda_n(L) = 0$ be its eigenvalues. The inequality $\lambda_1(L) \geq 1 + d_1$ is well known. The condition $\lambda_{n-1}(L) > 0$ characterizes the connected graphs.

The simple random walk on G is the process that jumps from a vertex i to any adjacent vertex j with equal transition probabilities $\frac{1}{d_i}$. In other words, this process is the Markov chain with transition matrix $P = D^{-1}A$ and its real eigenvalues are $1 = \lambda_1(P) > \lambda_2(P) \geq \cdots \geq \lambda_n(P) \geq -1$. For a bipartite graph, the spectrum of P is symmetric and, in particular, $\lambda_n(P) = -1$.

We now recall some notions about the majorization order and Schur-convexity (for more details see [16]). Let $\mathcal{D} = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq x_2 \geq \cdots \geq x_n\}$ and

$$\mathbf{s^0} = \mathbf{0},\ \mathbf{s^j} = \sum_{i=1}^{j} \mathbf{e^i},\ \mathbf{v^j} = \mathbf{s^n} - \mathbf{s^j} \quad j = 1, \dots, n$$

where $\mathbf{e^j}$, $j = 1, \dots, n$ are the fundamental vectors of $\mathbb{R}^n$. Given two vectors $\mathbf{y}, \mathbf{z} \in \mathcal{D}$, the majorization order $\mathbf{y} \trianglelefteq \mathbf{z}$ means:

$$\begin{cases} \langle \mathbf{y}, \mathbf{s^k} \rangle \leq \langle \mathbf{z}, \mathbf{s^k} \rangle, & k = 1, \dots, (n-1) \\ \langle \mathbf{y}, \mathbf{s^n} \rangle = \langle \mathbf{z}, \mathbf{s^n} \rangle \end{cases}$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{R}^n$. In the following we consider, without loss of generality, some subsets of

$$\Sigma_a = \mathcal{D} \cap \{\mathbf{x} \in \mathbb{R}^n_+ : \langle \mathbf{x}, \mathbf{s^n} \rangle = a\},$$

where $a \in \mathbb{R}$, $a > 0$. Given a closed subset $S \subseteq \Sigma_a$, a vector $\mathbf{x}^*(S) \in S$ is said to be maximal for S with respect to the majorization order if $\mathbf{x} \trianglelefteq \mathbf{x}^*(S)$ for each

$\mathbf{x} \in S$. Analogously, a vector $\mathbf{x}_*(S) \in S$ is said to be minimal for S with respect to the majorization order if $\mathbf{x}_*(S) \trianglelefteq \mathbf{x}$ for each $\mathbf{x} \in S$. Notice that the existence of maximal and minimal elements of S are ensured by the compactness of the upper and lower level sets:

$$U(\mathbf{z}) = \{\mathbf{x} \in S : \mathbf{z} \trianglelefteq \mathbf{x}\}, \ L(\mathbf{z}) = \{\mathbf{x} \in S : \mathbf{x} \trianglelefteq \mathbf{z}\}.$$

Remark 1 If we want to study the maximal and minimal elements of a subset S' of

$$\Sigma' = \{\mathbf{x} \in \mathbb{R}^n : x_1 \geq x_2 \geq \cdots \geq x_n \geq L, \langle \mathbf{x}, \mathbf{s^n} \rangle = a' > Ln\}$$

we can consider the change of variable $y_i = x_i - L$, $1 \leq i \leq n$. Then $\mathbf{y}$ belongs to a subset S of $\Sigma_{a'-Ln}$ with $(a' - Ln) > 0$ and it easy to verify that

$$x_*(S') = x_*(S) + L\mathbf{s^n}, \quad x^*(S') = x^*(S) + L\mathbf{s^n},$$

i.e. the maximal and minimal elements of S' can be easily deduced from the maximal and minimal elements of S adding to each component the constant L.

Definition 2 A symmetric function ϕ: $A \to \mathbb{R}$, $A \subseteq \mathbb{R}^n$, is said to be Schur-convex on A if $\mathbf{x} \trianglelefteq \mathbf{y}$ implies $\phi(\mathbf{x}) \leq \phi(\mathbf{y})$. If in addition $\phi(\mathbf{x}) < \phi(\mathbf{y})$ for $\mathbf{x} \trianglelefteq \mathbf{y}$ but $\mathbf{x}$ is not a permutation of $\mathbf{y}$, ϕ is said to be strictly Schur-convex on A. A function ϕ is (strictly) Schur-concave on A if $-\phi$ is (strictly) Schur-convex on A.

Thus, the set of S-convex functions preserves the ordering of majorization. In what follows we make use of some particular classes of functions yielding S-convex functions:

Proposition 3 *Let $I \subset \mathbb{R}$ be an interval and let $\phi(\mathbf{x}) = \sum_{i=1}^{n} g(x_i)$, where $g : I \to \mathbb{R}$. If g is strictly convex on I, then ϕ is strictly Schur-convex on $I^n = \underbrace{I \times \cdots \times I}_{n-times}$.*

It is worthwhile to consider the following result:

Proposition 4 *Let us consider two sets S'' and S', with $S'' \subseteq S'$, which admit maximal and minimal elements with respect to the majorization order. If ϕ is a strictly Schur-convex function, then*

$$\phi\left(\mathbf{x}^*\left(S''\right)\right) \leq \phi\left(\mathbf{x}^*\left(S'\right)\right)$$
$$\phi\left(\mathbf{x}_*\left(S'\right)\right) \leq \phi\left(\mathbf{x}_*\left(S''\right)\right)$$

and the equality holds if and only if $\mathbf{x}^*\left(S''\right) = \mathbf{x}^*\left(S'\right)$ and $\mathbf{x}_*\left(S''\right) = \mathbf{x}_*\left(S'\right)$.

In [3] the maximal and minimal elements of the set

$$S_a = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : M_i \geq x_i \geq m_i, \ i = 1, \ldots, n\}$$

where $M_1 \geq M_2 \geq \cdots \geq M_n$, $m_1 \geq m_2, \ldots \geq m_n$ were derived. For the sake of simplicity, we recall the main results given in [3]. Let $\mathbf{M} = [M_1, M_2, \ldots, M_n]^T$ and $\mathbf{m} = [m_1, m_2, \ldots, m_m]^T$, and denote by $\mathbf{x} \circ \mathbf{y}$ the Hadamard product of vectors $\mathbf{x}$ and $\mathbf{y}$. The integer part of the real number x is represented by $\lfloor x \rfloor$.

Theorem 5 *Let $k \geq 0$ be the smallest integer such that*

$$\left\langle \mathbf{M}, \mathbf{s^k} \right\rangle + \left\langle \mathbf{m}, \mathbf{v^k} \right\rangle \leq a < \left\langle \mathbf{M}, \mathbf{s}^{k+1} \right\rangle + \left\langle \mathbf{m}, \mathbf{v^{k+1}} \right\rangle,$$

and $\theta = a - \left\langle \mathbf{M}, \mathbf{s^k} \right\rangle - \left\langle \mathbf{m}, \mathbf{v^{k+1}} \right\rangle$. Then

$$\mathbf{x}^*(S_a) = \mathbf{M} \circ \mathbf{s^k} + \theta \mathbf{e}^{k+1} + \mathbf{m} \circ \mathbf{v^{k+1}}$$

From Theorem 5 a useful corollary follows

Corollary 6 (see [16]) *Let $0 \leq m < M$ and $m \leq \frac{a}{n} \leq M$. Given the subset*

$$S_1 = \Sigma_a \cap \left\{ \mathbf{x} \in \mathbb{R}^n : M \geq x_1 \geq x_2 \geq \cdots \geq x_n \geq m \right\}$$

we have

$$\mathbf{x}^*(S_1) = M\mathbf{s^k} + \theta \mathbf{e^{k+1}} + m\mathbf{v^{k+1}},$$

where $k = \left\lfloor \frac{a - nm}{M - m} \right\rfloor$ and $\theta = a - Mk - m\,(n - k - 1)$.

Theorem 7 *Let $k \geq 0$ and $d \geq 0$ be the smallest integers such that*

1) $k + d < n$

2) $m_{k+1} \leq \rho \leq M_{n-d}$ where $\rho = \dfrac{a - \langle \mathbf{m}, \mathbf{s^k} \rangle - \langle \mathbf{M}, \mathbf{v^{n-d}} \rangle}{n - k - d}$.

Then

$$\mathbf{x}_*(S_a) = \mathbf{m} \circ \mathbf{s^k} + \rho(\mathbf{s^{n-d}} - \mathbf{s^k}) + \mathbf{M} \circ \mathbf{v^{n-d}}.$$

From Theorem 7 the next corollaries follow

Corollary 8 (see [16]) *Let $0 \leq m < M$ and $m \leq \frac{a}{n} \leq M$. Then $x_*(S_1) = \frac{a}{n}\mathbf{s^n}$.*

Corollary 9 (see [3], Corollary 14) *Let us consider the set*

$$S_2^{[h]} = \Sigma_a \cap \{\mathbf{x} \in \mathbb{R}^n : x_i \geq \alpha,\ i = 1, \ldots, h,\ 1 \leq h \leq n,\ 0 < \alpha \leq \frac{a}{h}\}$$

Then

$$x_*(S_2^{[h]}) = \begin{cases} \dfrac{a}{n}\mathbf{s^n} & \text{if } \alpha \leq \dfrac{a}{n} \\ \alpha \mathbf{s^h} + \rho \mathbf{v^h} \text{ with } \rho = \dfrac{a - \alpha h}{n - h} & \text{if } \alpha > \dfrac{a}{n} \end{cases}.$$

Corollary 10 (see [3], Corollary 15) *Let* $1 \leq h \leq (n-1)$ *and* $0 < \alpha < a$. *Given the subset*

$$S_3^{[h]} = \Sigma_a \cap \left\{ \mathbf{x} \in \mathbb{R}^n : x_i \leq \alpha,\ i = h+1, \dots n \right\},$$

we have

$$x_*(S_3^{[h]}) = \begin{cases} \dfrac{a}{n}\mathbf{s^n} & \text{if } \alpha \geq \dfrac{a}{n} \\ \rho \mathbf{s^h} + \alpha \mathbf{v^h} \text{ with } \rho = \dfrac{a-(n-h)\alpha}{h} & \text{if } \alpha < \dfrac{a}{n} \end{cases}$$

3 Bounds for $K(G)$, revised and new

In addition to its original Definition (1), the Kirchhoff index has the expression

$$K(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i(L)}, \tag{2}$$

in terms of the eigenvalues of the Laplacian L (see [10,31]). If G is d-regular, then $L = dI - A,\ P = D^{-1}A = I - \frac{1}{d}L$ and

$$\lambda_{n-i+1}(P) = 1 - \frac{\lambda_i(L)}{d} \quad i = 1, \dots, n. \tag{3}$$

In this case, from (2), the alternative expression

$$K(G) = \frac{n}{d} \sum_{i=2}^{n} \frac{1}{1-\lambda_i(P)}$$

in terms of the eigenvalues of the transition matrix P holds (see [20]).

In case G is an arbitrary connected graph, we do not have such a compact expression, but still we have the bounds of Corollary 2 in [18]:

$$\left(\frac{n}{d_1}\right) \sum_{i=2}^{n} \left(\frac{1}{1-\lambda_i(P)}\right) \leq K(G) \leq \left(\frac{n}{d_n}\right) \sum_{i=2}^{n} \left(\frac{1}{1-\lambda_i(P)}\right). \tag{4}$$

All these expressions of $K(G)$ in terms of sums of inverses of eigenvalues can be used to find upper and lower bounds, as was done in [20] and [30].

In order to get new bounds for $K(G)$, we want to apply the majorization technique to the summations in (4), and we must deal with vectors arranged in nonincreasing order. With this aim, let us make a change of variable setting

$$\nu_i = 1 - \lambda_{n-i+1}(P),\ i = 1, \dots, (n-1).$$

For the vector $\nu \in \mathbb{R}^{n-1}$ we have

$$0 < \nu_{n-1} \leq \nu_{n-2} \leq \dots \leq \nu_1 \leq 2$$

and $\sum_{i=1}^{n-1} \nu_i = n$ since

$$\mathrm{tr}(P) = \sum_{i=1}^{n} \lambda_i(P) = 0 \Rightarrow \sum_{i=2}^{n} \lambda_i(P) = -1.$$

In order to tackle the inequalities in (4), we evaluate the extremal values of the Schur-convex function

$$f(\nu_1, \nu_2, \ldots, \nu_{n-1}) = \sum_{i=1}^{n-1} \frac{1}{\nu_i}. \tag{5}$$

Let us consider the sets

$$S = \{\nu \in \mathbb{R}^{n-1} : \sum_{i=1}^{n-1} \nu_i = n,\ \ 0 < \nu_{n-1} \le \nu_{n-2} \le \cdots \le \nu_1 \le 2\}$$

and

$$S_0 = \{\nu \in \mathbb{R}^{n-1} : \sum_{i=1}^{n-1} \nu_i = n,\ \ 0 \le \nu_{n-1} \le \nu_{n-2} \le \cdots \le \nu_1 \le 2\}$$

By Corollary 8 we know that the minimal element of S_0 with respect to the majorization order is given by

$$\left(\underbrace{\frac{n}{n-1}, \frac{n}{n-1}, \ldots, \frac{n}{n-1}}_{n-1}\right)$$

The function f attains its minimum at this point, with the minimum value given by $\frac{(n-1)^2}{n}$. Since the minimum point belongs also to S, we have $\min_S f = \min_{S_0} f = \frac{(n-1)^2}{n}$. By (4) we get

$$K(G) \ge \frac{(n-1)^2}{d_1} \tag{6}$$

which is the bound given in [18], Corollary 4. Notice that the lower bound is attained if and only if $G = K_n$, the complete graph on n vertices.

Analogously, we can obtain the bound for bipartite graphs. In this case $\lambda_n = -1$; this implies $\nu_1 = 2$, and so we face the set

$$S_0^b = \{\nu \in \mathbb{R}^{n-2} : \sum_{i=2}^{n-1} \nu_i = n-2,\ \ 0 \le \nu_{n-1} \le \nu_{n-2} \le \cdots \le \nu_2 \le 2\} \tag{7}$$

and the Schur-convex function

$$f^b(\nu_1, \ldots, \nu_{n-1}) = \frac{1}{2} + \sum_{i=2}^{n-1} \frac{1}{\nu_i}. \tag{8}$$

Since the minimal element with respect to the majorization order of S_0^b is given by

$$\left(\underbrace{1, 1, \ldots, 1}_{n-2}\right),$$

the function f attains its minimum at this point, with minimum value given by $\frac{2n-3}{2}$. Again by (4) we get the bound given in [18], Corollary 3:

$$K(G) \geq \frac{n(2n-3)}{2d_1}. \tag{9}$$

To obtain better bounds by means of majorization techniques, some subsets of S_0, or S_0^b in case of bipartite graphs, should be considered. Indeed, if we have more information on the localization of the eigenvalues $\lambda_i(P)$ of the transition matrix P, we can improve the lower bound by using Corollaries 9 and 10 and the upper bound of Corollary 6. In the following section we explore this possibility.

3.1 Lower bounds

We start analyzing some cases related to non-bipartite graphs.

Case 1: Assume we have the additional eigenvalue bound:

$$\lambda_n(P) \leq -\beta < 0.$$

We can say that

$$\nu_1 = 1 - \lambda_n(P) \geq 1 + \beta = \alpha \geq \frac{n}{n-1}.$$

In the case of $\alpha > \frac{n}{n-1}$ it is possible to get sharper bounds for the Kirchhoff index by applying Corollary 9. We consider the subset of S_0 given by

$$S_0^1 = \{\nu \in S_0 : \nu_1 \geq \alpha\}.$$

In order to compute the minimal element of S_0^1, we apply Corollary 9, obtaining

$$\left(\alpha, \underbrace{\frac{n-\alpha}{n-2}, \frac{n-\alpha}{n-2}, \ldots, \frac{n-\alpha}{n-2}}_{n-2}\right).$$

Thus the Schur-convex function f in (5) has minimum value in S_0^1 given by $\frac{1}{\alpha} + \dfrac{(n-2)^2}{n-\alpha}$ and this is also the minimum value of f on

$$S^1 = \{\nu \in S : \nu_1 \geq \alpha\}$$

We can thus infer

$$K(G) \geq \frac{n}{d_1}\left[\frac{1}{\alpha} + \frac{(n-2)^2}{n-\alpha}\right] \tag{10}$$

or, equivalently

$$K(G) \geq \frac{n}{d_1}\left[\frac{1}{1+\beta} + \frac{(n-2)^2}{n-1-\beta}\right]. \tag{11}$$

Case 2: Assume we know that

$$\lambda_2(P) \geq \beta > 0. \tag{12}$$

We can say that

$$\nu_{n-1} = 1 - \lambda_2(P) \leq 1 - \beta = \alpha < \frac{n}{n-1},$$

and we face the set

$$T_0^1 = \{\nu \in S_0 : \nu_{n-1} \leq \alpha\}.$$

By Corollary 10, the vector of minimal element of T_0^1 is given by

$$\left(\underbrace{\frac{n-\alpha}{n-2}, \frac{n-\alpha}{n-2}, \ldots, \frac{n-\alpha}{n-2}}_{n-2}, \alpha\right),$$

and, by the same arguments as before, we get the bound (10) which, in terms of β, is now given by

$$K(G) \geq \frac{n}{d_1}\left[\frac{1}{1-\beta} + \frac{(n-2)^2}{n-1+\beta}\right]. \tag{13}$$

We now investigate the case of bipartite graphs.

Since $\lambda_n(P) = -1$, case 1 is not significant and case 2 is equivalent to $\lambda_{n-1}(P) \leq -\beta < 0$, by the symmetry of the spectrum. Thus we only discuss a bound of type (12) and we face the set

$$S^b_{\lambda_2} = \left\{ \nu \in S^b_0 : \nu_{n-1} \le \alpha \right\}.$$

By Corollary 10, the vector of the minimal element of $S^b_{\lambda_2}$ is

$$\left(\underbrace{\frac{n-2-\alpha}{n-3}, \frac{n-2-\alpha}{n-3}, \ldots, \frac{n-2-\alpha}{n-3}}_{n-3}, \alpha \right), \tag{14}$$

and, taking into account (8), the corresponding bound is

$$K(G) \ge \frac{n}{d_1} \left[\frac{1}{2} + \frac{1}{\alpha} + \frac{(n-3)^2}{n-2-\alpha} \right],$$

which, in terms of β is

$$K(G) \ge \frac{n}{d_1} \left[\frac{\beta-3}{2(\beta-1)} + \frac{(n-3)^2}{n-3+\beta} \right]. \tag{15}$$

3.1.1 A general lower bound

Now we exploit Case 1 above in order to get a general lower bound. For every matrix P with real eigenvalues $\lambda_1(P) \ge \lambda_2(P) \ge \cdots \ge \lambda_n(P)$ the following inequality is well-known

$$\lambda_n(P) \le \mu - \frac{\sigma}{\sqrt{n-1}} \tag{16}$$

where $\mu = \frac{\text{tr}(P)}{n}$ and $\sigma^2 = \frac{\text{tr}(P^2)}{n} - \left(\frac{\text{tr}(P)}{n}\right)^2$ (see [27]).

If P is a transition matrix of the walk on a given connected graph G, we observe that $\text{tr}(P) = 0$ and $\text{tr}(P^2) = 2\sum_{(i,j)\in E} \dfrac{1}{d_i d_j}$. Then $\mu = 0$ and

$$\sigma^2 = \frac{2}{n} \sum_{(i,j)\in E} \frac{1}{d_i d_j} = \left(\frac{2}{n}\right) R_{-1}(G),$$

where $R_{-1}(G)$ is the general Randić index for $\alpha = -1$ (see [22] and [14]). Moreover, by the equality

$$\sigma^2 = \frac{\text{tr}(P^2)}{n} = \frac{1 + \sum_{i=2}^n \lambda_i^2}{n}$$

and the conditions on the eigenvalues of P, it easily follows that P has at least one eigenvalue whose absolute value is less than one. This gives $\sigma^2 < 1$. Notice that the upper bound $\sigma = 1$ is attained by any unconnected graph with an even number n of vertices and $\frac{n}{2}$ connected components, each of which of order two. In this case, the spectrum of P is $\left\{\underbrace{-1, -1, \ldots, -1}_{n/2}, \underbrace{1, 1, \ldots, 1}_{n/2}\right\}$ and consequently $\sigma = 1$.

It is also worth noting that $\frac{1}{n-1}$ is the minimal value attainable by σ^2 among all connected graph of order n. This follows by applying the majorization technique to the set

$$S = \left\{\lambda_2(P) \geq \lambda_3(P) \geq \cdots \lambda_n(P) \geq -1 : \sum_{i=2}^{n} \lambda_i(P) = -1\right\}.$$

Indeed, taking into account Remark 1, the minimal element of the set S is $\underbrace{\left(-\frac{1}{n-1}, \ldots, -\frac{1}{n-1}\right)}_{(n-1)times}$ which yields $\sigma = \frac{1}{\sqrt{n-1}}$. Notice that this value corresponds to the variance of the spectrum of the transition matrix P associated to the complete graph K_n.

Applying now (11) with $\beta = \frac{\sigma}{\sqrt{n-1}}$, we get the following

Proposition 11 *For any simple connected G*

$$K(G) \geq \frac{n}{d_1}\left[\frac{1}{1 + \frac{\sigma}{\sqrt{n-1}}} + \frac{(n-2)^2}{n - 1 - \frac{\sigma}{\sqrt{n-1}}}\right]. \tag{17}$$

The next proposition contributes to show that the new bound (17) always performs better than (6) except in the case where $G = K_n$ for which the two bounds coincide.

Proposition 12 *Let G be a simple connected graph on n vertices, with $n \geq 3$. The lower bound of $K(G)$ in (17) is an increasing function of σ for $\frac{1}{\sqrt{n-1}} \leq \sigma < 1$, where the equality in the left side holds if and only if $G = K_n$.*

Proof We have already noticed that $\frac{1}{\sqrt{n-1}} \leq \sigma < 1$, where the equality in the left side holds if and only if $G = K_n$. We proceed to show that the lower bound in (17) is an increasing function of σ. Denote by $x = 1 + \frac{\sigma}{\sqrt{n-1}}$ and consider the function

$$g(x) = \frac{n}{d_1}\left[\frac{1}{x} + \frac{(n-2)^2}{n-x}\right]$$

The first derivative of $g(x)$ is:

$$g'(x) = \frac{n}{d_1}\left[-\frac{1}{x^2} + \frac{(n-2)^2}{(n-x)^2}\right].$$

Table 1 Lower bounds for K_n, K_d and P_n

Graph	σ^2	bound (17)
K_n	$1/(n-1)$	$(n-1)$
K_d	$1/d$	$\frac{n}{d}\left(\frac{1}{1+\frac{1}{\sqrt{d(n-1)}}}+\frac{(n-2)^2}{n-1-\frac{1}{\sqrt{d(n-1)}}}\right)$
P_n	$\frac{n+1}{2n}$	$\frac{n}{2}\left(\frac{1}{1+\sqrt{\frac{n+1}{2n\,(n-1)}}}+\frac{(n-2)^2}{n-1-\sqrt{\frac{n+1}{2n\,(n-1)}}}\right)$

Then, it is easy to check that for $\dfrac{n}{n-1} \leq x < 1+\dfrac{1}{\sqrt{n-1}}$, g is an increasing function of x with minimum value attained at $x = \frac{n}{n-1}$ which corresponds to $G = K_n$. $\square$

Notice that, thanks to Proposition 4, the new bound (17) always performs better than (6). Indeed, for the complete graph K_n the bounds are equal, while for all other type of graphs, since $\sigma > \frac{1}{\sqrt{n-1}}$ by Proposition 12, the minimal element of the set S^1 majorizes the minimal element of the set S_0 and the bound improves.

In Table 1 we summarized the bounds of some particular classes of graphs with $n \geq 3$, where K_d is a $d-$regular graph and P_n a path on n vertices.

3.1.2 $d-$regular graphs

For a d-regular graph K_d we have further information about the eigenvalues of the transition matrix P. Indeed, by the fact that $\lambda_1(L) \geq 1+d$ and (3), we get $\lambda_n(P) \leq -\dfrac{1}{d}$, that is tighter than the bound $\lambda_n(P) \leq -\dfrac{\sigma}{\sqrt{n-1}} = -\dfrac{1}{\sqrt{d\,(n-1)}}$. Applying (11) we have:

$$K(G) \geq \frac{n}{d}\left[\frac{1}{1+\dfrac{1}{d}}+\frac{(n-2)^2}{n-1-\dfrac{1}{d}}\right] = \frac{n}{1+d}+\frac{n(n-2)^2}{nd-1-d}. \tag{18}$$

Notice that (18) is equal to (2) in [20], that corresponds to bound (1) in [30] for the particular case of d-regular graphs (Table 2).

Bound (18) can be strengthened if some tighter bounds on λ_1 are available. In [15], Corollary 9, it is shown that for a d-regular graph of diameter D

$$\lambda_1(L) \geq d+\frac{2D}{D+1}.$$

For $D > 1$ this bound is tighter than $\lambda_1(L) \geq d+1$, while the case $D = 1$ corresponds to the complete graph. For all graphs with a known diameter $D > 1$, we can thus improve bound (18) with the following:

Table 2 Numerical results for a 2-regular graph

n	Bound (18)	Bound (19)
3	2	2
4	4.533	4.629
5	8.095	8.25
6	12.667	13.008
7	18.242	18.667
8	24.821	25.448
50	1204.296	1211.784
75	2743.878	2755.514

Table 3 Numerical results for the d-cube, with $n = 2^d$, vertex degree and D equal to d

d	Bound (18)	Bound (19)
3	16.4	16.547
4	56.353	56.556
5	192.346	192.626

$$K(G) \geq \frac{n}{d}\left[\frac{1}{1+\frac{2D}{d(D+1)}} + \frac{(n-2)^2}{n-1-\frac{2D}{d(D+1)}}\right] \tag{19}$$

For a circle we know that $D = \dfrac{n}{2}$ for n even and $D = \dfrac{n-1}{2}$ for n odd. In Table 3 we summarize the results for two families of $d-$regular graph.

3.1.3 Using the Cheeger constant

Next we want to explore Case 2 where an information of the type in equation (12) is available. The following inequality is provided in [21]:

$$\lambda_2(P) \geq 1 - 2h, \tag{20}$$

where h is the Cheeger constant (for more details and in-depth analysis see [6]). When $1 - 2h > 0$, we are able to improve bounds (6) or (9). For instance let us consider a full binary tree of depth $d > 1$. It has $n = 2^{d+1} - 1$ vertices, $m = 2^{d+1} - 2$ edges and $d_1 = 3$. For such a tree $h = \dfrac{1}{2^{d+1} - 3}$ (see Example 3.3 in [21]), and bound (20) becomes

$$\lambda_2 \geq 1 - \frac{2}{2^{d+1} - 3}. \tag{21}$$

Since a tree is a bipartite graph, by (15) we have

$$K(G) \geq \frac{n}{3}\left[2^d - 1 + \frac{\left(2^{d+1}-3\right)(n-3)^2}{2^{d+1}(n-2)-3n+4}\right],$$

which, for $h < \frac{1}{2}$, improves (9), due to Proposition 4.

3.2 Upper bounds

Taking into account the domain of the function f we deal with, to get an upper bound we must obtain a maximal element with non-null components. To this end let us consider the set

$$S_\beta = \{\nu \in \mathbb{R}^{n-1} : \sum_{i=1}^{n-1} \nu_i = n, \quad 0 < \beta \leq \nu_{n-1} \leq \nu_{n-2} \leq \cdots \leq \nu_1 \leq 2\}.$$

For a d-regular graph, Palacios in [20] found the following upper bound where, for simplicity, we write $\lambda_2(P) = \lambda_2$:

$$K(G) \leq \frac{n(n-1)}{d(1-\lambda_2)}. \tag{22}$$

The quantity $(1-\lambda_2)$ is known as *spectral gap*. It is noteworthy to emphasize that the bound (22) holds in general, for $d = d_n$, as can be seen from the right inequality of (4).

It is possible to get an upper bound in terms of the spectral gap by applying our procedure. Taking $1 - \lambda_2 = \nu_{n-1}$, let us consider the set

$$S_{\lambda_2} = \{\nu \in \mathbb{R}^{n-2} : \sum_{i=1}^{n-2} \nu_i = (n-1+\lambda_2), \quad 0 < 1-\lambda_2 \leq \nu_{n-2} \leq \cdots \leq \nu_1 \leq 2\}.$$

From Corollary 6 the maximal element of S_{λ_2} is given by

$$\Big(\underbrace{2, 2, \ldots, 2}_{k}, \theta, \underbrace{1-\lambda_2, 1-\lambda_2, \ldots, 1-\lambda_2}_{n-k-3}\Big)$$

where

$$k = \left\lfloor \frac{\lambda_2(n-1)+1}{\lambda_2+1} \right\rfloor \quad \text{and} \quad \theta = \lambda_2(n-k-2) - k + 2.$$

Using (4) now we have proven the following

Proposition 13 *For any simple connected graph G*

$$K(G) \leq \frac{n}{d_n}\left(\frac{n-k-2}{1-\lambda_2}+\frac{k}{2}+\frac{1}{\theta}\right). \tag{23}$$

In particular, for a bipartite graph, since $\lambda_n = -1$, we deal with the set:

$$S^b_{\lambda_2} = \{\nu \in \mathbb{R}^{n-3} : \sum_{i=2}^{n-2} \nu_i = (n-3+\lambda_2),\ \ 0 < 1-\lambda_2 \leq \nu_{n-2} \leq \cdots \leq \nu_2 \leq 2\}.$$

By Corollary 6 the maximal element of $S^b_{\lambda_2}$ is

$$\left(\underbrace{2, 2, \ldots, 2}_{k}, \theta, \underbrace{1-\lambda_2, 1-\lambda_2, \ldots, 1-\lambda_2}_{n-k-4}\right)$$

where

$$k = \left\lfloor \frac{\lambda_2\,(n-2)}{\lambda_2+1} \right\rfloor \quad \text{and} \quad \theta = \lambda_2\,(n-k-3) - k + 1.$$

The upper bound (4) is given in this case by

$$K(G) \leq \frac{n}{d_n}\left(\frac{1}{2}+\frac{n-k-3}{1-\lambda_2}+\frac{k}{2}+\frac{1}{\theta}\right). \tag{24}$$

In what follows we consider some examples of particular graphs whose spectral gap is well-known. It is worth noting that, due to Proposition 4, our bounds always perform equal or better than the bounds provided in [20].

1. **The complete graph**
   For a complete graph K_n, we know that $\lambda_2 = -\dfrac{1}{n-1}$. In this case

$$k = 0 \text{ and } \theta = \frac{n}{n-1}$$

and (23) becomes

$$K(G) \leq \frac{n}{d}\left(\frac{(n-2)\,(n-1)}{n}+\frac{n-1}{n}\right) = \frac{(n-1)^2}{d} = (n-1)$$

giving the exact value of the index.

Table 4 Numerical results for the star graph $K_{1,n-1}$

n	Bound (22)	Bound (26)	Exact value (2)
2	2	1	1
3	6	4.5	4
4	12	10	9
5	20	17.5	16
6	30	27	25
7	42	38.5	36

2. **The complete bipartite graph**
   For a complete bipartite graph $K_{r,s}$ graph, with $r < s$, $n = r + s$ we know that $\lambda_2 = 0$ and

$$S^b_{\lambda_2} = \left\{ v \in \mathbb{R}^{n-3} : \sum_{i=2}^{r+s-2} v_i = r + s - 3, \quad 1 \leq v_{n-2} \leq \cdots v_2 \leq 2 \right\}.$$

By simple computations we get:

$$k = 0 \text{ and } \theta = 1.$$

The vector of minimal elements in this case is

$$\left(\underbrace{1, 1, \ldots, 1}_{r+s-3} \right)$$

and by (24) the bound is

$$K(G) \leq \frac{r+s}{r} (r + s - 3/2). \tag{25}$$

For $r = s = n$ we get the real value of the index $K(G) = 4n - 3$.

2.a **The star graph**
   The star graph is the particular case of complete bipartite graph $K_{1,n-1}$ and, by considering $n = s + 1$, $r = 1$, (25) becomes

$$K(G) \leq n (n - 3/2). \tag{26}$$

We provide some numerical results in order to compare bounds (26) and (22) which, as observed before, holds in general when $d = d_n$, and the actual value of the index. The results are shown in Table 4.

Table 5 Numerical results for the n-cycle

n	Bound (22)	Bound (23)	Exact value (2)
3	2	2	2
4	6	5	5
5	14.472	10.031	10
6	30	18	17.5
7	55.775	33.259	28
8	95.598	50.538	42

Table 6 Numerical results for the d-cube

d	Bound (22)	Bound (23)	Exact value (2)
2	6	5	5
3	28	20.66	19.33
4	120	84.66	68.67
5	496	334.5	236.53

3. **The *n*-cycle**
   The n-cycle graph is a particular type of d-regular graph, specifically it is a 2-regular graph, whose second largest eigenvalue is $\lambda_2 = \cos\left(\frac{2\pi}{n}\right)$. The numerical results are summarized in the Table 5, for $n \geq 3$.

4. **The *d*-cube**
   The second largest eigenvalue of the d-cube is $\lambda_2 = \frac{d-2}{d}$. We show the results in Table 6.

3.3 The degree-Kirchhoff index

To conclude, we want to point out that our work thus far can be applied to another index related to the Kirchhoff index. The *degree-Kirchhoff index* was proposed by Chen and Zhang in [5], defined as

$$K'(G) = \sum_{i<j} d_i d_j R_{ij}.$$

This index was looked at in [18], where the following expression in terms of the eigenvalues of the transition matrix P was given:

$$K'(G) = 2|E| \sum_{j=2}^{n} \frac{1}{1-\lambda_j}. \tag{27}$$

Furthermore, it was shown that

$$K^{'}(G) \geq \frac{2|E|(n-1)^2}{n}, \tag{28}$$

which is basically bound (6), after replacing $\frac{n}{d_1}$ with $2|E|$. An upper bound of order n^5 for this index that is attained (up to the constant of the leading term) by the barbell graph was provided in [18] also. With electrical network techniques, the lower bound was improved in [19] to

$$K^{'}(G) \geq 2|E| \left(n - 2 + \frac{1}{d_1 + 1} \right). \tag{29}$$

It is clear, by looking at the expression (27), that we can obtain new upper and lower bounds for $K^{'}(G)$ by exchanging in (17), (18), (23) and (24) the terms $\frac{n}{d_1}$ or $\frac{n}{d_n}$ with $2|E|$, and by exchanging $K(G)$ with $K^{'}(G)$. Of all those bounds, perhaps the only one worth mentioning explicitly is in the following

Proposition 14 *For any simple connected G we have*

$$K^{'}(G) \geq 2|E| \left[\frac{1}{1 + \frac{\sigma}{\sqrt{n-1}}} + \frac{(n-2)^2}{n - 1 - \frac{\sigma}{\sqrt{n-1}}} \right]. \tag{30}$$

This bound improves (29) if G has at least one vertex with degree $n-1$.

Here σ is defined as in Proposition 10. The only thing left to show is that (30) improves (29) under the given condition, which is clear because in that case (29) becomes (28), which is always less than (30), by the arguments after Proposition 12.

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