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More on Topological Indices and Their Reciprocals

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Abstract

We show how Schwitzer inequality allows us to find inequalities relating an additive descriptor of the form $D_p(G) = \sum_{i=1}^{N} c_i^p$ to its reciprocal $D_{-p}(G) = \sum_{i=1}^{N} c_i^{-p}$. We look at three cases (the inverse degree, the Kirchhoff, and the multiplicative degree-Kirchhoff indices) where $p = 1$ and where, of the two $D_1(G)$ and $D_{-1}(G)$, one is known in closed form, therefore allowing to find an upper bounds for the other.

1 Introduction

Let $G = (V, E)$ be a simple, connected, undirected graph where $V = \{v_1, ..., v_n\}$ is the set of vertices and E the set of edges. We denote by $\Delta = d_1 \geq d_2 \geq ... \geq d_n = \delta$ the degrees of the vertices of G. It is well known that $\sum_{i=1}^{n} d_i = 2|E|$. Let $A(G)$ be the adjacency matrix of G and $D(G)$ be the diagonal matrix of vertex degrees. The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of G, with eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, while $\mathcal{L}(G) = D(G)^{-1/2} L(G) D(G)^{-1/2}$ is known as the normalized Laplacian, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} > \lambda_n = 0$. For more details on graph theory we refer the reader to [9].

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In this article we are interested in topological descriptors of a graph G with the form

$$D_p(G) = \sum_{i=1}^{N} c_i^p, \tag{1}$$

where the c_is are some positive parameters associated to G, and p is an arbitrary real number. Sometimes these descriptors arise as generalizations of other descriptors which were originally thought of as particular cases of p. An example of these is the general first Zagreb index

$$M_1^p(G) = \sum_{i=1}^{n} d_i^p,$$

which generalizes the first Zagreb index, obtained when $p = 2$. The reader should consult the survey [8] for a discussion of this and several other indices.

Sometimes the descriptors that we will look at do not generalize former descriptors, but still have the form (1), for example

$$s_p(G) = \sum_{i=1}^{n-1} \mu_i^p,$$

where the μ_is are the non-zero Laplacian eigenvalues of G, and

$$s_p^*(G) = \sum_{i=1}^{n-1} \lambda_i^p,$$

where the λ_is are the non-zero normalized Laplacian eigenvalues of G. These latter descriptors were introduced in [20]. One particular variant of $s_{-1}(G)$ is the Kirchhoff index

$$K_f(G) = ns_{-1}(G),$$

whose expression in terms of the Laplacian eigenvalues was found in [7] and [21]. This index also has a more physical definition, put forward in [10], as

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

where R_{ij} is the effective resistance, computed with Ohm's laws, between vertices i and j. Another electrical index that we will touch upon in this article, introduced in [2], is the multiplicative degree-Kirchhoff index:

$$K_f^*(G) = \sum_{i<j} d_i d_j R_{ij}.$$

Depending on the topological index studied, the index of the summation in (1) can run in one of the sets $\{1, 2, \ldots, n\}$, or $\{1, 2, \ldots, n-1\}$, or E, or all the pairs of indices i, j such that $i < j$, conveniently ordered. In this article N will be either n or $n-1$, and the context will make clear which case is being considered. In what follows, using Schweitzer inequality, we derive a relation involving $D_p(G)$ and its reciprocal $D_{-p}(G)$, and then focus on some particular cases. We refer the reader to our previous work [14], for other relationships between additive indices of the form (1) found using Radon's inequality.

2 Schweitzer inequality and its applications to descriptors

We start off with the main tool of this note, Schweitzer inequality, first shown in [15] and usually found in the context of Probability Theory and Statistics (see [5] [19]; in the latter there is a history of the inequality):

Lemma 1. *For all* $0 < m \leq x_i \leq M$ *we have*

$$\sum_{i=1}^{n} x_i \sum_{i=1}^{n} \frac{1}{x_i} \leq \frac{n^2(m+M)^2}{4mM}. \tag{2}$$

The equality holds whenever $m = x_i = M$ *for all* i*, or whenever* n *is* *even and*

$$x_1 = \cdots = x_{\frac{n}{2}} = m \quad \text{and} \quad x_{(\frac{n}{2}+1)} = \cdots = x_n = M.$$

In [11], Lupaş showed the following refinement of Schweitzer inequality:

Lemma 2. *For all* $0 < m \leq x_i \leq M$ *and* n *is odd we have*

$$\sum_{i=1}^{n} x_i \sum_{i=1}^{n} \frac{1}{x_i} \leq \frac{n^2(M+m)^2 - (M-m)^2}{4mM}. \tag{3}$$

The equality holds when $m = x_i = M$ *for all* i*, or when the smallest* $\frac{n-1}{2}$ *of the numbers* $x_1, \ldots x_n$ *are equal to* m*, the largest* $\frac{n-1}{2}$ *are equal to* M*, and the middle* x_i *is equal to either* m *or* M*.*

Now we can prove the following

Theorem 1. *For any descriptor* $D_p(G)$ *of the form given in (1), we have*

$$N^2 \leq D_p(G) D_{-p}(G) \leq N^2 \frac{(m+M)^2}{4mM}. \tag{4}$$

Both equalities are attained in case $m = c_i^p = M$ *for all* $1 \leq i \leq N$*. Also, the right inequality is attained if* n *is even and the first* $\frac{n}{2}$ *of the* c_i^p*s are equal to* m *and the other* $\frac{n}{2}$ *of the* c_i^p*s are equal to* M*.*

Also, if n *is odd we have*

$$N^2 \leq D_p(G) D_{-p}(G) \leq \frac{N^2(M+m)^2 - (M-m)^2}{4mM}. \tag{5}$$

Both equalities are attained in case $m = c_i^p = M$ *for all* $1 \leq i \leq N$*. Also, the right equality is attained if the first* $\frac{n-1}{2}$ *of the* c_i^p*s are equal to* m*, the last* $\frac{n-1}{2}$ *of the* c_i^p*s are equal to* M*, and the middle* c_i^p *is either* m *or* M*.*

Proof. The left inequalities hold by the arithmetic-harmonic-mean inequality. The right inequalities are shown taking $x_i = c_i^\alpha$ in (2) and (3)
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Note. In [6] the authors use the same idea of relating indices and their reciprocals with the help of Schweitzer inequality. However, the inequality is incorrectly used and all their purported lower bounds are actually upper bounds. Also, as shown above, their claim that the equality is attained if and only if all the terms in the summation are equal is inexact.

In what follows we will obtain a series of corollaries from theorem 1. We start with $M_1^{-1}(G)$, more commonly known as the inverse degree index $ID(G)$, and notice that its reciprocal is $M_1^1(G) = 2|E|$. We get the following

Corollary. *For any n-vertex graph G we have*

$$\frac{n^2}{2|E|} \leq ID(G) \leq \frac{n^2(\Delta+\delta)^2}{8|E|\Delta\delta}, \tag{6}$$

where both equalities are attained for regular graphs, and the right equality is also attained by biregular graphs such that n is even, half the vertices have degree δ and the other half have degree Δ.

Also, if n is odd we have

$$\frac{n^2}{2|E|} \leq ID(G) \leq \frac{n^2(\Delta+\delta)^2 - (\Delta-\delta)^2}{8|E|\Delta\delta}, \tag{7}$$

where both equalities are attained for regular graphs, and also the right equality is attained by biregular graphs such that $\frac{n-1}{2}$ vertices have degree δ and $\frac{n+1}{2}$ vertices have degree Δ, or biregular graphs such that $\frac{n+1}{2}$ vertices have degree δ and $\frac{n-1}{2}$ vertices have degree Δ.

The index $ID(G)$ has been extensively studied, and our bounds (6) and (7) are at least not comparable to those found in the literature: for instance, those in [3] are not attained by our biregular graphs, and the one similar to our (7) found in [4]:

$$ID(G) \leq \frac{n(\Delta+\delta) - 2|E|}{\Delta\delta}, \tag{8}$$

is better than ours for biregular graphs with a different distribution of degrees than those in corollary 1. However, for the unicyclic graphs G_n consisting of a triangle with a $n-3$ -long path graph attached to one of the vertices on the triangle, we have that the bound (8) becomes $\frac{2n}{3}$, which is the same value obtained for our bound (6) for n even, but it is worse than our (7) for n odd, which becomes $\frac{2n}{3} - \frac{1}{6n}$.

Now we study the Kirchhoff index $K_f(G) = n\sum_{i=1}^{n-1} \frac{1}{\lambda_i}$, and with the help of the well known fact that $\sum_{i=1}^{n-1} \lambda_i = 2|E|$, we produce bounds that to the best of our knowledge are new.

Corollary. *For all G we have*

$$\frac{n(n-1)^2}{2|E|} \leq K_f(G) \leq \frac{n(n-1)^2(m+M)^2}{8|E|mM}, \tag{9}$$

where m is the smallest eigenvalue and M is the largest eigenvalue of the Laplacian matrix. Both equalities holds when all the eigenvalues are the same, which is the case of the complete graph. Also, the right equality holds when there are only two nonzero eigenvalues with the same multiplicity and n is odd. Also, when n is even and there are only two nonzero eigenvalues, whose multiplicities differ by 1, we get the refinement

$$\frac{n(n-1)^2}{2|E|} \leq K_f(G) \leq \frac{n\left[(n-1)^2(m+M)^2 - (M-m)^2\right]}{8|E|mM}, \tag{10}$$

The cases where the right inequalities in (9) and (10) become equalities, i.e., where the graphs have only two nonzero eigenvalues with multiplicities either equal or differing by one, are abundant, and the subject of study in [16] and [19]. For instance, in the former reference they mention two graphs on 16 vertices with Laplace spectra $\{0, 8^7, 4^8\}$ and $\{0, 8^8, 4^7\}$, that attain the right equality in (10). It is also simple to verify that (10) is attained by $K_{1,3}$ and $K_{2,2}$, whereas (9) is attained by $K_{1,2}$.

We now obtain bounds for the multiplicative degree-Kirchhoff index $K_f^*(G)$ using the index $s_1^*(G)$ and its reciprocal $s_{-1}^*(G)$, defined above, and for which it is well known that (see [1], for instance)

$$s_1^*(G) = n, \tag{11}$$

and

$$s^*_{-1}(G) = \frac{1}{2|E|} K^*_f(G). \tag{12}$$

An application of theorem 1 yields the following

Corollary. *For all G we have*

$$\frac{2|E|(n-1)^2}{n} \leq K^*_f(G) \leq \frac{2|E|(n-1)^2(m+M)^2}{4nmM}, \tag{13}$$

where m is the smallest eigenvalue and M is the largest eigenvalue of the normalized Laplacian matrix. Both equalities hold when all the eigenvalues are the same, which is the case of the complete graph. Also, the right equality holds when there are only two nonzero eigenvalues with the same multiplicity and n is odd. Also, when n is even and there are only two nonzero eigenvalues, whose multiplicities differ by 1 we get the refinement

$$\frac{2|E|(n-1)^2}{n} \leq K^*_f(G) \leq \frac{2|E|\left[(n-1)^2(m+M)^2 - (M-m)^2\right]}{4nmM}. \tag{14}$$

As in the case of corollary 2, the cases where the right equalities in (13) and (14) are attained correspond to graphs with exactly two nonzero normalized Laplacian eigenvalues. These graphs have been studied in [17], and out of those, we are interested in the ones whose multiplicities are equal or differ by 1. In that regard, we need this definition: a *cone* over a graph G is a graph obtained by adjoining a new vertex to all vertices of G, i.e., it is a graph with a vertex with degree $n-1$. Then, as stated in [17], a cone over a disjoint union of an isolated vertex and a strongly regular graph with parameters (n, k, λ, μ) with $n = 2k+1$, $k = 2\mu$ and $\lambda = \mu - 1$ has exactly two nonzero normalized Laplacian eigenvalues: $\frac{n \pm \sqrt{n-2}}{n-1}$, each with multiplicity $\frac{n-1}{2}$, and thus all these graphs attain the equality in (13). Also, $K_{1,2}$ attains the equality in (13) and $K_{1,3}$ and $K_{2,2}$ attain the equality in (14).

A final observation regarding the joint behavior of the two Kirchhoffian indices studied in this article: the left inequalities of (9) and (13) allow us to conclude that

Corollary. *for all G we have*

$$(n-1)^4 \leq K_f(G) K_f^*(G).$$

The equality is attained by the complete graph.

Finding the graph that attains the maximum value of the product $K_f(G)K_f^*(G)$ seems to be a rather hard problem (see [13]).

References

[1] M. Bianchi, A. Cornaro, J. L. Palacios, A. Torriero, Bounding the sum of powers of normalized Laplacian eigenvalues of graphs through majorization methods, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 707–716.

[2] H. Chen, F. Zhang, Resistance distance and the normalized Laplacian spectrum, *Discr. Appl. Math,* **155** (2007) 654–661.

[3] K. C. Das, K. Xu, J. Wang, On inverse degree and topological indices of graphs, *Filomat* **30** (2016) 2111–2120.

[4] S. Elumalai, S. M. Hosamani, T. Mansour, M. A. Rostami, More on inverse degree and topological indices of graphs, *Filomat* **32** (2018) 165–178.

[5] S. Filipowski, New bounds for the mean and the variance, *Contrib. Math.* **7** (2023) 48–52.

[6] I. Gutman, B. Furtula, I. Redžepović, On topological indices and their reciprocals, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 287–297.

[7] I. Gutman, B. Mohar, The quasi-Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985.

[8] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graphs Comb.* (2018) `https://doi.org/10.1016/akcej.2018.05.002`.

[9] F. Harary, *Graph Theory*, Addison Wesley, Reading, 1969.

[10] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem* **12** (1993) 81–95.

[11] A. Lupaş, A remark on the Schweitzer and Kantorovich inequalities, *Publ. Elektrotehn. Fak. Univ. Beogradu Ser. Mat. i Fiz.* **383** (1972) 13–14.

[12] E. D. Molina, J. M. Rodríguez, J. L. Sánchez, J. M. Sigarreta, Applications of the inverse degree index to molecular structures, *J. Math. Chem* (2023) `https://doi.org/10.1007/s10910-023-01526-z`.

[13] J. L. Palacios, Some interplay of the three Kirchhoffian indices, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 199–206.

[14] J. L. Palacios, Applications of Radon's inequalities to generalized topological descriptors, *Contrib. Math.* **8** (2023) 30–37.

[15] P. Schweitzer, An inequality about the arithmetic mean, *Math, Phys. Lapok* **23** (1914) 257–261.

[16] E. R. Van Dam, W. H. Haemers, Graphs with constant μ and $\bar{\mu}$, *Discr. Math.* **182** (1998) 293–307.

[17] E. R. Van Dam, G. R. Omidi, Graphs whose normalized Laplacian has three eigenvalues, *Lin. Algebra Appl.* **435** (2011) 2560–2569.

[18] Y. Wang, Y. Fan, Y. tan, On graphs with three distinct Laplacian eigenvalues, *Appl. Math. J. Chinese U. Ser. B* **22** (2007) 478–484.

[19] G. S. Watson, G. Alpargu, G. P. H. Styan, Some comments on six inequalities associated with the inefficiency of ordinary least squares with one regressor, *Lin. Algebra Appl.* **264** (1997) 13–53.

[20] B. Zhou, On a sum of powers of the Laplacian eigenvalues of a graphs,*Lin. Algebra Appl.* **429** (2008) 2239–2246.

[21] H. Y. Zhu, D. J. Klein, I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Compt. Sci.* **36** (1996) 420–428.