

Comparing Laplacian Energy and Kirchhoff Index

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Abstract

Let G be a connected graph of order n and size m with Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n = 0$. The Laplacian energy and the Kirchhoff index of G are defined as $LE = \sum_{i=1}^n |\mu_i - \frac{2m}{n}|$ and $Kf = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$, respectively. We show that $Kf < LE$ holds for one class of graphs, and find another class for which $Kf > LE$.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$, $|E(G)| = m$. Let $A(G)$ be the $(0, 1)$ -adjacency matrix of G and $D(G)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. Denote by $Spec(G) = (\mu_1, \mu_2, \dots, \mu_n)$ the spectrum of $L(G)$, i.e., the Laplacian spectrum of G , and recall that $n \geq \mu_1 \geq \mu_2 \geq \dots \geq \mu_n = 0$.

The *Laplacian energy* of the graph G is defined as [16]

$$LE = LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right|. \quad (1)$$

For its basic mathematical properties, including various lower and upper bounds, see [7, 8, 16, 22, 24] and especially the most recent works [4, 9–11] and the book [15].

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Let σ ($1 \leq \sigma \leq n$) be the largest positive integer such that $\mu_\sigma \geq \frac{2m}{n}$. Then from (1), we have

$$LE(G) = 2 S_\sigma(G) - \frac{4m\sigma}{n} \tag{2}$$

where

$$S_\sigma(G) = \sum_{i=1}^{\sigma} \mu_i.$$

In the 1990s, Klein and Randić [17] considered the *resistance distance* between two vertices of a (connected) graph, defined as the electric resistance in a network corresponding to that graph, in which the resistance between any two adjacent nodes is unity. Then, in analogy to the classical Wiener index, the sum of resistance distances between all pairs of vertices was considered [1, 17] and was named *Kirchhoff index*.

The Kirchhoff index has a very nice connection with Laplacian eigenvalues, namely [14, 25]

$$Kf = Kf(G) = n \sum_{k=1}^{n-1} \frac{1}{\mu_k}.$$

The Kirchhoff index found noteworthy applications in chemistry, as a molecular structure descriptor [1, 5], and many of its mathematical properties have been established [2, 12, 19–21, 23].

Interestingly, until now the relation between the two Laplacian–spectrum based graph invariants LE and Kf did not attract much attention [6, 13, 18]. In this paper we prove that $LE > Kf$ for some classes of graphs and $LE < Kf$ for some other classes.[†]

2 Main Result

In this section we compare the Laplacian energy and the Kirchhoff index. For this we need the following two auxiliary lemmas:

Lemma 1. [3] *Let G be a simple graph with at least one edge. Then $\mu_1 = \mu_2 = \dots = \mu_{n-1}$ if and only if $G \cong K_n$.*

Lemma 2. [6] *Let G be a graph of order n with m edges. Then $\mu_1(G) \leq m + 1$.*

[†]The results presented here were originally part of Ref. [6]. After the paper [6] received positive referee reports, based on a suggestion of the Editor, the results on the comparison of LE and Kf were edited out. Namely, the Editor “did not want to promote more papers on this topic”, maintaining that there already were too many publications on graph spectra and energy, whereas our results would stimulate the production of more such articles.

For $G \cong K_n$ ($n \geq 2$), $LE(G) = 2(n-1) > n-1 = Kf(G)$.

For $G \cong K_{1,n-1}$ ($n > 2$), $LE(G) = 2n-4 + \frac{4}{n} < n(n-2) + 1 = Kf(G)$.

Therefore $LE(G)$ and $Kf(G)$ are incomparable on the class of general graphs. On the other hand, we have the following result:

Theorem 1. *Let G be a graph obtained by deleting p edges from the complete graph K_n ($n \geq 11$). If $0 \leq p \leq n/2$, then $Kf(G) < LE(G)$.*

Proof. Let \bar{G} denote the complement of the graph G . Let \bar{m} be the number of edges of \bar{G} . Then $0 \leq \bar{m} = p \leq n/2$.

Let k be the number of connected components of \bar{G} . Let n_i and m_i ($i = 1, 2, \dots, k$) be the number of vertices and edges in the i -th connected component of \bar{G} . Then $m_i \geq n_i - 1$, $i = 1, 2, \dots, k$. Thus

$$p = \sum_{i=1}^k m_i \geq \sum_{i=1}^k (n_i - 1) = n - k, \quad \text{that is, } k \geq n - p.$$

Since k is the number of connected components of \bar{G} , it follows that n is a Laplacian eigenvalue of G with multiplicity $k - 1$, that is, n is a Laplacian eigenvalue of G with multiplicity at least $n - p - 1$.

By Lemma 2, $\mu_1(\bar{G}) \leq p + 1$, that is, $\mu_{n-1}(G) \geq n - p - 1 \geq n/2 - 1$. Using these results, we arrive at

$$\begin{aligned} Kf(G) &= \sum_{i=1}^{n-p-1} \frac{n}{\mu_i(G)} + \sum_{i=n-p}^{n-1} \frac{n}{\mu_i(G)} \\ &< (n-p-1) + \sum_{i=n-p}^{n-1} \frac{n}{n-p-1} = n-p-1 + \frac{np}{n-p-1}. \end{aligned}$$

Since $2m + 2\bar{m} = n(n-1)$, we have $2m + 2p = n(n-1)$. Using this, we get

$$\begin{aligned} LE(G) &= \mu_1 + \sum_{i=2}^{n-1} \left| \mu_i - \frac{2m}{n} \right| = \mu_1 + \sum_{i=2}^{n-1} \left| \mu_i - (n-1) + \frac{2p}{n} \right| \\ &= n + \left(1 + \frac{2p}{n} \right) (n-p-2) + \sum_{i=n-p}^{n-1} \left| \mu_i - (n-1) + \frac{2p}{n} \right| \\ &\geq n + \left(1 + \frac{2p}{n} \right) (n-p-2). \end{aligned}$$

Consider the function

$$h(p) = n - 1 + \frac{2p}{n} (n - p - 2) - \frac{np}{n - p - 1}, \quad 1 \leq p \leq n/2.$$

Then

$$h''(p) = -\frac{4}{n} - \frac{2n(n-1)}{(n-p-1)^3} < 0.$$

Therefore $h(p)$ is a decreasing function on $1 \leq p \leq n/2$ and thus

$$h(p) \geq h(n/2) = \frac{n(n-6)}{2(n-2)} - 3 > 0 \quad \text{as } n \geq 11.$$

From the above results, it follows $LE(G) - Kf(G) > h(p) > 0$, that is, $Kf(G) < LE(G)$. ■

Theorem 2. *Let G be a connected graph of order n . If $m \leq n\sqrt{\frac{n-1}{8}}$, then $Kf(G) > LE(G)$.*

Proof. Recalling the definition of S_σ , observe that

$$S_\sigma = \sum_{i=1}^{\sigma} \mu_i \leq \sum_{i=1}^{n-1} \mu_i = 2m.$$

By (2) and $\sigma \geq 1$, the above result yields

$$LE(G) = \sum_{i=1}^n \left| \mu_i - \frac{2m}{n} \right| = 2S_\sigma - \frac{4m\sigma}{n} \leq \frac{4m(n-1)}{n}.$$

By the arithmetic–harmonic–mean inequality, for $m \leq n\sqrt{\frac{n-1}{8}}$ we have

$$\begin{aligned} Kf(G) &= \sum_{i=1}^{n-1} \frac{n}{\mu_i} \geq \frac{n(n-1)^2}{2m} \\ &\geq \frac{4m}{n}(n-1) \geq LE(G). \end{aligned} \tag{3}$$

By the arithmetic–harmonic–mean inequality, the equality holds in (3) if and only if $\mu_1 = \mu_2 = \dots = \mu_{n-1}$, that is, if $G \cong K_n$, by Lemma 1. Since $m \leq n\sqrt{\frac{n-1}{8}}$, we conclude that $Kf(G) > LE(G)$. ■

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