

On extended connectivity indices

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Abstract Bonchev and Kier proposed sometime ago the extended connectivity indices, which may be used in structure–property–activity modeling. We establish some properties, mainly various lower and upper bounds for the first extended zeroth-order connectivity index ${}^0\chi_1$ and the first extended first-order connectivity index ${}^1\chi_1$.

Keywords Connectivity index · Extended connectivity indices · Properties · Zagreb indices

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$ [1]. For $v \in V(G)$, $\Gamma(v)$ denotes the set of its (first) neighbors in G and the degree of v is $d_v = |\Gamma(v)|$. Denote by uv or vu the edge of G connecting vertices u and v .

The zeroth-order connectivity index ${}^0\chi(G)$ and the first-order connectivity index (also called the Randić index [2,3] or simply the connectivity index [4]) ${}^1\chi(G)$ of the graph G are defined respectively as [5,6]

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$$\begin{aligned}
 {}^0\chi(G) &= \sum_{v \in V(G)} d_v^{-1/2}, \\
 {}^1\chi(G) &= \sum_{uv \in E(G)} (d_u d_v)^{-1/2}.
 \end{aligned}$$

${}^1\chi$ is one of the most popular descriptors and have found countless QSPR and QSAR applications, see, e.g. [7–11]. ${}^0\chi$ is also used to develop structure-based correlations for physical properties, see, e.g. [12].

In [13], Bonchev and Kier proposed the extended connectivity indices ${}^0\chi_k, {}^1\chi_k$. For a nonnegative integer k , the k th extended zeroth-order connectivity index ${}^0\chi_k(G)$ and the k th extended first-order connectivity index ${}^1\chi_k(G)$ of the graph G are defined respectively as

$$\begin{aligned}
 {}^0\chi_k(G) &= \sum_{v \in V(G)} \binom{k}{d_v}^{-1/2}, \\
 {}^1\chi_k(G) &= \sum_{uv \in E(G)} \binom{k}{d_u \cdot d_v}^{-1/2},
 \end{aligned}$$

where ${}^0d_v = d_v$ and ${}^k d_v = \sum_{u \in \Gamma(v)} {}^{k-1}d_u$ for $k \geq 1$. Evidently, ${}^0\chi_0 = {}^0\chi, {}^1\chi_0 = {}^1\chi$. Note that in [13], the cases $k = 1, 2, 3, 4$ were considered. Toropov et al. [14] showed that the extended connectivity indices may be used for structure–property studies.

In this report, we establish some properties, mainly various lower and upper bounds for the first extended zeroth-order connectivity index

$${}^0\chi_1(G) = \sum_{v \in V(G)} \binom{1}{d_v}^{-1/2}$$

and the first extended first-order connectivity index

$${}^1\chi_1(G) = \sum_{uv \in E(G)} \binom{1}{d_u \cdot d_v}^{-1/2}.$$

For simplicity, let $D_v = {}^1d_v = \sum_{u \in \Gamma(v)} d_u$.

2 Results

Let G be a connected simple graph. Recall that the first $M_1(G)$ and the second $M_2(G)$ Zagreb indices are defined respectively as [15–18]

$$\begin{aligned}
 M_1(G) &= \sum_{v \in V(G)} d_v^2, \\
 M_2(G) &= \sum_{uv \in E(G)} d_u d_v.
 \end{aligned}$$

Let K_n be the complete graph with n vertices [1]. Let K_{n_1, n_2, \dots, n_s} be the complete s -partite graph [1] with respectively n_i vertices in i th partite sets for $i = 1, 2, \dots, s$. Let $S_n = K_{1, n-1}$ be the star with n vertices [1].

For any non-isolated vertex $v \in V(G)$, we have $D_v \geq d_v$ with equality if and only if any neighbor of v has degree one. Thus, if G has no isolated vertices, then ${}^0\chi_1(G) \leq {}^0\chi_0(G)$ and ${}^1\chi_1(G) \leq {}^1\chi_0(G)$ with either equality if and only if G is the vertex-disjoint union of complete graphs with two vertices. It follows that for any connected graph G with at least three vertices, ${}^0\chi_1(G) < {}^0\chi_0(G)$ and ${}^1\chi_1(G) < {}^1\chi_0(G)$.

In the following we establish further properties of ${}^0\chi_1$ and ${}^1\chi_1$. We first consider ${}^0\chi_1$.

Proposition 1 *Let G be a graph with n vertices and no isolated vertices. Then*

$${}^0\chi_1(G) \geq \sqrt{\frac{n^3}{M_1(G)}}$$

with equality if and only if all D_v are equal.

Proof By the Cauchy–Schwarz inequality, we have

$${}^0\chi_1(G) = \sum_{v \in V(G)} \frac{1}{\sqrt{D_v}} \geq \frac{n^2}{\sum_{v \in V(G)} \sqrt{D_v}} \geq \frac{n^2}{\sqrt{n \sum_{v \in V(G)} D_v}}$$

with equalities if and only if all D_v are equal. Note that

$$\sum_{v \in V(G)} D_v = \sum_{v \in V(G)} \sum_{u \in \Gamma(v)} d_u = \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} d_u = \sum_{u \in V(G)} d_u \sum_{v \in \Gamma(u)} 1 = M_1(G).$$

The result follows. □

By Proposition 1, upper bounds for $M_1(G)$ may be used to deduce lower bounds for ${}^0\chi_1(G)$. Note that various upper bounds for $M_1(G)$ have been known, see, e.g. [18–23]. As an example, we give the following proposition. The Moore graphs of diameter 2 are the regular graphs of diameter 2 and girth 5. They are pentagon, Petersen graph, Hoffman–Singleton graph, and possibly a 57-regular graph with $57^2 + 1 = 3250$ vertices whose existence is still an open problem, see, e.g. [21, 24].

Proposition 2 *Let G be a triangle- and quadrangle-free graph with n vertices and no isolated vertices. Then*

$${}^0\chi_1(G) \geq \frac{n}{\sqrt{n-1}}$$

with equality if and only if G is the star or a Moore graph of diameter 2.

Proof Since G is triangle- and quadrangle-free, we have [21]

$$M_1(G) \leq n(n - 1)$$

with equality if and only if G is the star or a Moore graph of diameter 2. Since the Moore graphs of diameter 2 are regular, all D_v are equal. Now the result follows from Proposition 1 easily. \square

Let G be a tree with $n \geq 2$ vertices. Then by Proposition 2, ${}^0\chi_1(G) \geq n/\sqrt{n - 1}$ with equality if and only if $G = S_n$.

Now we consider properties of ${}^1\chi_1$.

Proposition 3 *Let G be a graph with n vertices and no isolated vertices. Then*

$${}^1\chi_1(G) \leq \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{D_v}$$

with equality if and only if $D_u = D_v$ for any pair of adjacent vertices u and v . Moreover, if G possesses m edges, maximum vertex degree Δ and minimum vertex degree δ such that $2m - (n - 1)\Delta + (\Delta - 1)\delta > 0$, then

$${}^1\chi_1(G) \leq \frac{m}{2m - (n - 1)\Delta + (\Delta - 1)\delta}$$

with equality if and only if G is a regular graph. \square

Proof It is easily seen that

$$\begin{aligned} {}^1\chi_1(G) &= \frac{1}{2} \left[\sum_{uv \in E(G)} \left(\frac{1}{D_u} + \frac{1}{D_v} \right) - \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{D_u}} - \frac{1}{\sqrt{D_v}} \right)^2 \right] \\ &= \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{D_v} - \frac{1}{2} \sum_{uv \in E(G)} \left(\frac{1}{\sqrt{D_u}} - \frac{1}{\sqrt{D_v}} \right)^2 \leq \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{D_v} \end{aligned}$$

with equality if and only if $D_u = D_v$ for any pair of adjacent vertices u and v .

Since $D_v = \sum_{u \in \Gamma(v)} d_u$, we have $D_v \geq 2m - d_v - (n - 1 - d_v)\Delta = 2m - (n - 1)\Delta + (\Delta - 1)d_v$ with equality for the vertex v if and only if either $d_v = n - 1$ or $d_u = \Delta$ for any vertex u (different from v) that is not adjacent to v , and thus with equality for all vertices of G if and only if either $G = K_n$ or any pair of non-adjacent vertices has equal degree Δ , i.e., G is regular since Δ is the maximum vertex degree.

Note that $\sum_{v \in V(G)} d_v = 2m$ and that if G is a regular graph then $D_u = D_v$ for any pair of vertices u and v . Thus

$$\begin{aligned} {}^1\chi_1(G) &\leq \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{2m - (n-1)\Delta + (\Delta-1)d_v} \\ &\leq \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{2m - (n-1)\Delta + (\Delta-1)\delta} \\ &= \frac{m}{2m - (n-1)\Delta + (\Delta-1)\delta} \end{aligned}$$

with equalities if and only if G is a regular graph. \square

Let G be a graph with n vertices. From Proposition 3, we have

$${}^1\chi_1(G) \leq \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{D_v} \leq \frac{1}{2} \sum_{v \in V(G)} \frac{d_v}{d_v} \leq \frac{n}{2}$$

with equalities if and only if G has no isolated vertex and $D_v = d_v$ for any vertex v , i.e., G is the vertex-disjoint union of complete graphs with two vertices.

Proposition 4 *Let G be a graph with n vertices, m edges, minimum vertex degree δ and no isolated vertices. Then*

$${}^1\chi_1(G) \geq \frac{m^{3/2}}{\left[m(2m - (n-1)\delta)^2 + (2m - (n-1)\delta)(\delta-1)M_1(G) + (\delta-1)^2M_2(G) \right]^{1/2}} \quad (1)$$

with equality if and only if G is a regular graph or the star.

Proof By the Cauchy–Schwarz inequality, we have

$${}^1\chi_1(G) = \sum_{uv \in E(G)} (D_u D_v)^{-1/2} \geq \frac{m^2}{\sum_{uv \in E(G)} (D_u D_v)^{1/2}} \geq \frac{m^2}{\left(m \sum_{uv \in E(G)} D_u D_v \right)^{1/2}}$$

with equalities if and only if $D_u = D_v$ for any pair of adjacent vertices u and v . For any vertex v , $D_v \leq 2m - d_v - (n - d_v - 1)\delta = 2m - (n-1)\delta + (\delta-1)d_v$ with equality if and only if either $d_v = n-1$ or $d_u = \delta$ for any vertex u (different from v) that is not adjacent to v . Note that $\sum_{uv \in E(G)} (d_u + d_v) = M_1(G)$. Thus

$$\begin{aligned} \sum_{uv \in E(G)} D_u D_v &\leq \sum_{uv \in E(G)} [2m - (n - 1)\delta + (\delta - 1)d_u][2m - (n - 1)\delta + (\delta - 1)d_v] \\ &= m [2m - (n - 1)\delta]^2 + [2m - (n - 1)\delta] (\delta - 1) \sum_{uv \in E(G)} (d_u + d_v) \\ &\quad + (\delta - 1)^2 \sum_{uv \in E(G)} d_u d_v \\ &= m [2m - (n - 1)\delta]^2 + [2m - (n - 1)\delta] (\delta - 1)M_1(G) \\ &\quad + (\delta - 1)^2 M_2(G). \end{aligned}$$

Now (1) follows and equality holds in (1) if and only if $D_u = D_v$ for any pair of adjacent vertices u and v and $D_v = 2m - (n - 1)\delta + (\delta - 1)d_v$ for any vertex v , or equivalently G is a regular graph if $\delta > 1$ and G is the star if $\delta = 1$. \square

The clique number of a graph G is the number of vertices in a largest complete subgraph of G , denoted by $\omega(G)$. We will use a theorem of Motzkin and Straus [25], which we state a somewhat differently from the original version.

Lemma 5 ([25]) *Let G be a graph and let $x_v \geq 0$ for $v \in V(G)$ with $\sum_{v \in V(G)} x_v = 1$. Then $\sum_{uv \in E(G)} x_u x_v \leq \frac{\omega(G)-1}{2\omega(G)}$ with equality if and only if the subgraph induced by the vertices $v \in V(G)$ with $x_v > 0$ is a complete $\omega(G)$ -partite graph such that the sum of the x_v 's in each part is the same.*

Proposition 6 *Let G be a graph with $m \geq 1$ edges and clique number ω . Then*

$${}^1\chi_1(G) \geq \frac{\sqrt{2\omega m}}{\sqrt{\omega - 1}M_1(G)} \tag{2}$$

with equality when G has no isolated vertices if and only if G is a regular complete ω -partite graph.

Proof From the proof of Proposition 4,

$${}^1\chi_1(G) \geq \frac{m^{3/2}}{\left[\sum_{uv \in E(G)} (D_u D_v) \right]^{1/2}}.$$

Note that $\sum_{v \in V(G)} D_v = M_1(G)$. For $v \in V(G)$, let $x_v = \frac{D_v}{M_1(G)}$ if $d_v > 0$ and $x_v = 0$ if $d_v = 0$. Then $x_v \geq 0$ for $v \in V(G)$ with $\sum_{v \in V(G)} x_v = 1$. By Lemma 5,

$$\sum_{uv \in E(G)} \frac{D_u}{M_1(G)} \cdot \frac{D_v}{M_1(G)} \leq \frac{\omega - 1}{2\omega}$$

i.e.,

$$\sum_{uv \in E(G)} D_u D_v \leq \frac{\omega - 1}{2\omega} M_1(G)^2$$

and then (2) follows.

Suppose that G has no isolated vertices and that equality holds in (2). Note that $x_v > 0$ for any $v \in V(G)$. By Lemma 5, G is a complete ω -partite graph, say $G = K_{n_1, \dots, n_\omega}$, and the sum of the x_v 's in each partite set is the same. Then $n_i \sum_{k \neq i} n_k (n - n_k) = n_j \sum_{k \neq j} n_k (n - n_k)$, i.e., $(n_i - n_j) [\sum_{k \neq i, j} n_k (n - n_k) + n_i n_j] = 0$, i.e., $n_i = n_j$ for any $1 \leq i < j \leq \omega$. Conversely, it is easily checked that (2) is an equality for a regular complete ω -partite graph. \square

Let G be a K_{r+1} -free graph with n vertices, $m \geq 1$ edges, where $2 \leq r \leq n - 1$. Then $\omega(G) \leq r$ and by Proposition 6,

$${}^1\chi_1(G) \geq \frac{\sqrt{2rmm}}{\sqrt{r-1}M_1(G)}$$

with equality when G has no isolated vertices if and only if G is a regular complete r -partite graph. Recall that $M_1(G) \leq \frac{2r-2}{r}nm$ (see [23]). Then

$${}^1\chi_1(G) \geq \frac{r\sqrt{rm}}{(r-1)\sqrt{2(r-1)n}}$$

with equality when G has no isolated vertices if and only if G is a regular complete r -partite graph.

The vertex-disjoint union of graphs G and H is denoted by $G \cup H$, pG denotes the vertex-disjoint union of p copies of G .

Proposition 7 *Let G be a $K_{1,1,s+1}$ - and $K_{2,t+1}$ -free graph with $n \geq \max\{s+3, t+3\}$ vertices, $m \geq 1$ edges, where $0 \leq s \leq t$. Then*

$${}^1\chi_1(G) \geq \frac{m^{3/2}}{[t^2(n-1)^2m + t(n-1)(s+1-t)M_1(G) + (s+1-t)^2M_2(G)]^{1/2}} \quad (3)$$

with equality if and only if G is a strongly regular graph (each pair of adjacent vertices in G has exactly s common neighbors and each pair of non-adjacent vertices has exactly t common neighbors), or $s = t = 0$ and $G = aK_2 \cup bK_1$ with $n = 2a + b$, or $s = 0, t = 1$ and $G = S_n$.

Proof From the proof of Proposition 4,

$${}^1\chi_1(G) \geq \frac{m^{3/2}}{\left(\sum_{uv \in E(G)} D_u D_v\right)^{1/2}}.$$

It is known [23] that $D_v \leq (s + 1 - t)d_v + t(n - 1)$ with equality if and only if v has exactly s neighbors in common with any of its neighbor and has exactly t neighbors in common with any vertex (different from v) non-adjacent to it. Thus

$$\begin{aligned} \sum_{uv \in E(G)} D_u D_v &\leq \sum_{uv \in E(G)} [(s + 1 - t)d_u + t(n - 1)][(s + 1 - t)d_v + t(n - 1)] \\ &= t^2(n - 1)^2 m + t(n - 1)(s + 1 - t) \sum_{uv \in E(G)} (d_u + d_v) \\ &\quad + (s + 1 - t)^2 \sum_{uv \in E(G)} d_u d_v \\ &= t^2(n - 1)^2 m + t(n - 1)(s + 1 - t)M_1(G) + (s + 1 - t)^2 M_2(G). \end{aligned}$$

Now (3) follows and equality holds in (3) if and only if (i) $D_u = D_v$ for any pair of adjacent vertices u and v , and (ii) each pair of adjacent vertices in G has exactly s common neighbors and each pair of non-adjacent vertices in G has exactly t common neighbors. Recently there is a result obtained by Gera and Shen [26]: If G is an irregular graph in which each pair of adjacent vertices has exactly s common neighbors and each pair of non-adjacent vertices in G has exactly t common neighbors, then either $t = 0$ and $G = aK_{s+2} \cup bK_1$ with $n = a(s + 2) + b$ or $t = 1$ and $G = K_1 \vee aK_{s+1}$ is the graph obtained by adding all edges between a vertex and vertices of aK_{s+1} with $n = a(s + 1) + 1$. It follows that (ii) is equivalent to G is a strongly regular graph, or $s = t = 0$ and $G = aK_2 \cup bK_1$ with $n = 2a + b$, or $s = t = 1$ and G is the graph W_n obtained by adding $\frac{n-1}{2}$ independent edges to the star with odd n , or $s = 0, t = 1$ and $G = S_n$. Note that (i) does not hold for W_n when $s = t = 1$. Now the result follows easily. \square

If G is a quadrangle-free graph with $n \geq 4$ vertices and $m \geq 1$ edges, then by Proposition 7 with $s = t = 1$,

$${}^1\chi_1(G) > \frac{m^{3/2}}{[(n - 1)^2 m + (n - 1)M_1(G) + M_2(G)]^{1/2}}.$$

The inequality is strict because by the Friendship theorem [27, 28], the graph in which each pair of (distinct) vertices in G has exactly one common neighbor must be W_n .

If G is a quadrangle-free graph with $n \geq 4$ vertices and $m \geq 1$ edges, then by Proposition 7 with $s = 0, t = 1$,

$${}^1\chi_1(G) \geq \frac{m}{n - 1}$$

with equality if and only if G is a strongly regular graph in which each pair of adjacent vertices in G has no common neighbors and each pair of non-adjacent vertices has exactly 1 common neighbor, or $G = S_n$. A strongly regular graph with n vertices in which each pair of adjacent vertices in G has no common neighbors and each pair of non-adjacency vertices has exactly 1 common neighbor is regular of degree $\sqrt{n - 1}$,

and thus it is a Moore graph of diameter 2. Thus the bound for ${}^1\chi_1(G)$ is attained if and only if G is a Moore graph of diameter 2, or $G = S_n$.

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