The connectivity index of a weighted graph

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Abstract

Let $G$ be a simple graph and consider the $m$-connectivity index $\chi_m(G) = \sum_{i_1, i_2, \ldots, i_m, 1} 1/\sqrt{d_{i_1} d_{i_2} \cdots d_{i_m, 1}}$, where $i_1 - i_2 - \cdots - i_{m, 1}$ runs over all paths of length $m$ in $G$ and $d_i$ denotes the degree of the vertex $i$. We find upper bounds for $\chi_m(G)$ using the eigenvalues of the Laplacian matrix of an associated weighted graph. The method provides also lower bounds for $\chi(G)$. © 1998 Elsevier Science Inc. All rights reserved.

1. Introduction

Let $G$ be a simple graph, that is, $G$ does not have loops or multiple edges. Let \{1, \ldots, n\} be the set of vertices of $G$ and $d_i$ denotes the degree of the vertex $i$.

In 1975, Randić [5] introduced the 1-connectivity index (now called also Randić index) as

$$\chi(G) = \sum_{i - j} 1/\sqrt{d_i d_j},$$

where $i - j$ runs over all the edges of $G$. This index has been successfully related to physical and chemical properties of organic molecules. Indeed, if $G$ is the molecular graph of a saturated hydrocarbon (that is, the vertices of $G$ represent
the carbon atoms of the molecules and the edges, the electronic bonds), then there is a strong correlation between $\chi(G)$ and the boiling point of the substance. See Refs. [3,4,6].

Of interest also in molecular graph theory are the higher connectivity indices. For $m \geq 1$, we consider the $m$-connectivity index as

$$m\chi(G) = \sum_{i_1 - i_2 - \cdots - i_{m+1}} \frac{1}{\sqrt{d_{i_1}d_{i_2} \cdots d_{i_{m+1}}}},$$

where $i_1 - i_2 - \cdots - i_{m+1}$ runs over all paths (that is, $i_{j-1} \neq i_{j+1}$ for $2 \leq j \leq m$ and possibly $i_s = i_t$ for $1 \leq s < t < m$) of length $m$ in $G$. The purpose of this work is to find bounds for the values of $m\chi(G)$, $m \geq 1$.

**Theorem 1.** Let $G$ be a simple graph with vertices 1, ..., $n$. Let $d_{\text{max}}$ be the maximal value of $d_i$ ($1 \leq i \leq n$) and $\Delta = (d_{\text{max}} - 1)/\sqrt{d_{\text{max}}}$. Then

$$m\chi(G) \leq \frac{\Delta^{m-1}}{2} [n^{(m)}(G) + c^{(m)}(G)],$$

where $n^{(m)}(G)$ is the number of vertices $i$ in $G$ such that there is at least one path of length $m$ starting at $i$ and $c^{(m)}(G)$ counts those $i$ which accept a path of length $m$ from $i$ to $i$.

For the proof of Theorem 1 we introduce in Section 2 the concept of the connectivity index of a weighted graph and use the theory of weighted Laplacian matrices. If $G$ is a simple graph with vertices 1, ..., $n$, the Laplacian $L$ of $G$ is the $n \times n$ matrix with entries

$$L(i,j) = \begin{cases} 1 & \text{if } i = j \text{ and } d_i \neq 0, \\ -\frac{1}{\sqrt{d_i}} & \text{if } i \neq j, \\ 0 & \text{else}. \end{cases}$$

If $G$ is connected, then $L$ has eigenvalues $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1}$. (See [1].) Then we may show the following more precise bounds for $\chi(G)$.

**Theorem 2.** Let $G$ be a simple connected graph with vertices 1, ..., $n$. Then

$$\frac{1}{2} [n - \lambda_{n-1}(n - \kappa)] \leq \chi(G) \leq \frac{1}{2} [n - \lambda_1(n - \kappa)],$$

where $\kappa$ is a graph invariant defined as $\kappa = (\sum_{i=1}^n \sqrt{d_i})^2 / (\sum_{i=1}^n d_i)$. Moreover, $\kappa \leq n$ and $\chi(G) = n/2$ (and $\kappa = n$) if and only if $G$ is regular.

We shall present the proof of Theorem 2 in Section 2 and that of Theorem 1 in Section 3.
2. Weighted graphs

(1) Let $G$ be a graph, possibly with loops but not multiple edges. Let $V = \{1, \ldots, n\}$ be the set of vertices of $G$. A pair $(G, w)$ is a weighted graph if $w: V \times V \to \mathbb{R}$ is a function satisfying: $w(i, j) = w(j, i)$; $w(i, j) \geq 0$ and $w(i, j) > 0$ if and only if $i - j$ is an edge in $G$, for all $i, j \in V$.

Following Ref. [1], we introduce the following concepts: $d_i = \sum_{j \neq i} w(i, j)$ is the degree of a vertex $i$; $\text{vol}(G, w) = \sum_{i=1}^{n} d_i$ the volume of the weighted graph $(G, w)$; the Laplacian $\mathcal{L}$ of $(G, w)$ the $n \times n$ matrix whose $(i, j)$-entry is:

$$
\mathcal{L}(i, j) = \begin{cases} 
1 - \frac{w(i, j)}{d_i} & \text{if } i = j \text{ and } d_i \neq 0, \\
- \frac{w(i, j)}{\sqrt{d_i d_j}} & \text{if } i - j \text{ and } i \neq j \text{ in } G, \\
0 & \text{else}.
\end{cases}
$$

Then $\lambda_0 = 0$ is an eigenvalue of $\mathcal{L}$ with eigenvector $v_0 = (\sqrt{d_1}, \ldots, \sqrt{d_n})$. If $G$ is connected $\lambda_0$ is an eigenvalue of multiplicity one.

Assume $G$ is connected. The other eigenvalues of $\mathcal{L}$ are $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1}$. Since $\mathcal{L}$ is symmetric, by Rayleigh–Ritz’ Theorem (see for example Ref. [2]), we have

$$
\lambda_1 = \inf_{0 \neq v \in \mathbb{R}^n} \frac{v^T \mathcal{L} v}{\|v\|^2} = \inf_{u} \frac{\sum_{i \neq j} (u(i) - u(j))^2 w(i, j)}{\sum_{i=1}^{n} u(i)^2 d_i},
$$

where $u$ runs over all vectors in $\mathbb{R}^n$ with $\sum_{i=1}^{n} u(i) d_i = 0$; and

$$
\lambda_{n-1} = \sup_{0 \neq v \in \mathbb{R}^n} \frac{v^T \mathcal{L} v}{\|v\|^2}.
$$

(2) We introduce the graph invariant $\kappa (= \kappa(G, w))$ as

$$
\kappa = \frac{(\sum_{i=1}^{n} \sqrt{d_i})^2}{\text{vol}(G, w)}.
$$

In fact, $n - \kappa$ is a measure of the deviation of $\{\sqrt{d_1}, \ldots, \sqrt{d_n}\}$ from the mean $d = (1/n)\sum_{i=1}^{n} \sqrt{d_i}$. We have the following lemma.

**Lemma.** (a) If $G$ is connected, then $(n^2/\text{vol}(G, w)) \leq \kappa \leq n$;

(b) $n - \kappa = \frac{n}{\text{vol}(G, w)} \sum_{i=1}^{n} (\sqrt{d_i} - d)^2$;

(c) $\kappa = n$ if and only if $(G, w)$ is regular, that is, $d_i = d_j$ for every $1 \leq i, j \leq n$.

**Proof.** (a) Since $\sqrt{d_i d_j} \leq \frac{1}{2} (d_i + d_j)$, then

$$
\left(\sum_{i=1}^{n} \sqrt{d_i}\right)^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \sqrt{d_i d_j} \leq \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (d_i + d_j) = n \sum_{i=1}^{n} d_i.
$$
(b) Trivially, \( \sum_{i=1}^{n} (\sqrt{d_i} - \bar{d})^2 = \sum_{i=1}^{n} d_i - (1/n)(\sum_{i=1}^{n} \sqrt{d_i})^2 \).

(c) Obvious. \( \square \)

(3) The connectivity index of the weighted graph \((G, w)\) is defined as:

\[
\chi(G, w) = \sum_{i \neq j} \frac{w(i, j)}{\sqrt{d_i d_j}}.
\]

We obtain the following relations of \( \chi(G, w) \) and the eigenvalues of the Laplacian of \((G, w)\).

**Theorem.** Let \((G, w)\) be a weighted connected graph. Assume \(\{1, \ldots, n\}\) is the set of vertices of \(G\) and \(0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1}\) the eigenvalues of the Laplacian \(\mathcal{L}\) of \((G, w)\). Then

\[
\frac{1}{2} \left[ n + \sum_{i=1}^{n} \frac{w(i, i)}{d_i} - \lambda_{n-1}(n - \kappa) \right] \leq \chi(G, w) \leq \frac{1}{2} \left[ n + \sum_{i=1}^{n} \frac{w(i, i)}{d_i} - \lambda_1(n - \kappa) \right]
\]

Moreover, \( \chi(G, w) = (1/2) \left[ n + \sum_{i=1}^{n} w(i, i)/d_i \right] \) if and only if \((G, w)\) is regular.

**Proof.** We consider the quadratic form \(x^\mathcal{L}x\) associated to the symmetric matrix \(\mathcal{L}\). Since all the eigenvalues of \(\mathcal{L}\) are non-negative, then Jacobi criterion says that \(x^\mathcal{L}x\) is non-negative. In particular, if \(v_1 = (1, \ldots, 1)\) is the vector with 1 in all its entries, then

\[
0 \leq v_1^\mathcal{L}v_1 = \sum_{i=1}^{n} \left( 1 - \frac{w(i, i)}{d_i} \right) - 2 \sum_{i=1}^{n} \frac{w(i, j)}{\sqrt{d_id_j}} = n + \sum_{i=1}^{n} \frac{w(i, i)}{d_i} - 2\chi(G, w).
\]

If \((G, w)\) is regular, then \(v_0 = \bar{d}v_1\) and \(v_1^\mathcal{L}v_1 = 0\). Moreover, by (2) of Section 1, \(\kappa = n\) and therefore the inequalities of the statement are satisfied.

Assume \((G, w)\) is not regular. Then \(v_0\) and \(v_1\) are linearly independent and \(0 \neq \tilde{v}_1 = v_1 - (v_0 \cdot v_1'/\|v_0\|^2)v_0\) is orthogonal to \(v_0\). A simple calculation shows that \(\|\tilde{v}_1\|^2 = n - \kappa\). Moreover, since \(x^\mathcal{L}x\) is non-negative and \(\mathcal{L}v_0 = 0\), then \(\mathcal{L}\tilde{v}_1 = v_1^\mathcal{L}v_1\). Hence,

\[
\lambda_1 \leq \frac{v_1^\mathcal{L}v_1}{n - \kappa} \leq \lambda_{n-1}
\]

and the result immediately follows. \( \square \)

(4) Clearly, Theorem 2 in Section 1 is a particular case of (3) of Section 1 when \(G\) is a connected simple graph with weights defined as \(w(i, j) = 1\) if \(i - j\) in \(G\) and 0 else.
3. The connectivity index of simple graphs

(1) Let $G$ be a simple graph with vertices $1, \ldots, n = n(G)$. We assume that every connected component of $G$ has at least two vertices (equivalently, $d_i \geq 1$ for all $1 \leq i \leq n$). We want to find a priori bounds for $m\chi(G)$, $m \geq 1$.

Let $m \geq 1$. We introduce a weighted graph $(G^{(m)}, w^{(m)})$ in the following way: the vertices of $G^{(m)}$ are those $1 \leq i \leq n$ such that there is at least one path $i = i_1 - i_2 - \cdots - i_{m+1}$ in $G$; there is an edge $i - j$ in $G^{(m)}$ if there is a path $i = i_1 - i_2 - \cdots - i_{m+1} = j$ and

$$w^{(m)}(i, j) = \sum_{i = i_1 - i_2 - \cdots - i_{m+1} = j} (d_{i_2} \cdots d_{i_{m+1}})^{-1/2},$$

where the sum runs over all paths in $G$ of length $m$ between $i$ and $j$. We denote by $n^{(m)}(G) := n(G^{(m)})$ the number of vertices of $G^{(m)}$. Let $d_i^{(m)}$ be the degree of a vertex $i$ in the weighted graph $(G^{(m)}, w^{(m)})$.

**Lemma.** For $1 \leq i \leq n^{(m)}(G)$, we have $\delta^{m-1}d_i \leq d_i^{(m)} \leq (d_{\max} - 1)/\sqrt{d_{\max}}$ and $\delta = (d_{\min}' - 1)/\sqrt{d_{\min}'}$ for $d_{\min}' = \min\{d_i : 2 \leq d_i\}$.

**Proof.** We may assume that $m \geq 2$. By definition,

$$d_i^{(m)} = \sum_{i = j} w^{(m)}(i, j) = \sum_{i = i_1 - \cdots - i_{m+1} = j} (d_{i_2} \cdots d_{i_{m+1}})^{-1/2} = \sum_{i = i_1 - \cdots - i_{m}} (d_{i_2} \cdots d_{i_{m}})^{-1/2} d_i^{(m)} (d_{i_{m+1}} - 1),$$

the last equality due to the fact that there are $d_{i_{m+1}} - 1$ choices for $j$ once $i = i_1 - \cdots - i_{m}$ is fixed. Since $\delta \leq d_i^{1/2}(d_i - 1) \leq \Delta$ for any vertex $x$ with $d_i \geq 2$, then

$$\delta d_i^{(m-1)} \leq d_i^{(m)} \leq \delta d_i^{(m-1)} \Delta,$$

and the result follows by induction. \(\Box\)

(2) The connectivity index $\chi(G^{(m)}, w^{(m)})$ of the weighted graph $(G^{(m)}, w^{(m)})$ and $m\chi(G)$ are related in the following simple way.

**Proposition.** $(1/\Delta)^{m-1}m\chi(G) \leq \chi(G^{(m)}, w^{(m)}) \leq (1/\delta)^{m-1}m\chi(G)$.

**Proof.** By definition

$$\chi(G^{(m)}, w^{(m)}) = \sum_{i,j} w^{(m)}(i, j) (d_i^{(m)} d_j^{(m)})^{-1/2} = \sum \left[ \frac{d_id_j}{d_i^{(m)} d_j^{(m)}} \right]^{1/2} (d_i d_{i_2} \cdots d_{i_{m+1}})^{-1/2}$$

where the last sum runs over all paths $i = i_1 - i_2 - \cdots - i_m - i_{m+1} = j$ of length $m$ in $G$. The inequalities follow from (1) of Section 3. \(\Box\)
Proof of Theorem 1. We define \((G^{(m)}, w^{(m)})\) as above. By (3) of Section 1,
\[
\chi(G^{(m)}, w^{(m)}) \leq \frac{1}{2} \left[ n(G^{(m)}) + \sum_i \frac{w^{(m)}(i,i)}{d_i^{(m)}} \right] \leq \frac{1}{2} [n^{(m)}(G) + c^{(m)}(G)].
\]
Then (2) of Section 3 yields the desired bound. \(\square\)

Some examples. (a) Consider the graph \(G\) (See Fig. 1(a)). Then the eigenvalues of the Laplacian \(\mathcal{L}\) are 0, 1, 3/2 and 2. Since \(G\) is regular, then \(\chi(G) = 2\) and \(\kappa = 4\). Since \(\delta = \Delta = 1/\sqrt{2}\), then by (2) \(\chi(G) = \left(\frac{1}{\sqrt{2}}\right)^{m-1} \chi(G^{(m)}, w^{(m)})\) for all \(m \geq 1\).

For \(G^{(2)}\), the weight function is \(w^{(2)}(1,3) = \sqrt{2} = w^{(2)}(2,4)\). Then \(\chi(G^{(2)}, w^{(2)}) = 2\) and \(\chi(G) = \sqrt{2}\). For \(G^{(3)} = G\), the weight function is \(w^{(3)}(i,j) = 1/2\) if \(i \neq j\). Then \(\chi(G^{(3)}, w^{(3)}) = 2\) and \(\chi(G) = 1\). For \(G^{(4)}\) the weight function is \(w^{(4)}(i,i) = 1/\sqrt{2}\). Then \(\chi(G^{(4)}, w^{(4)}) = 4\) and \(\chi(G) = \sqrt{2}\). Observe that \(n^{(4)}(G) = 4\) and the bound given in Theorem 1 for \(\chi(G)\) is reached.

(b) We consider the graph \(G\). It is not hard to see (as mentioned in Ref. [1]) that \(\lambda_1 = 1/2\) and \(\lambda_6 = 3/2\), where \(0 = \lambda_0 < \lambda_1 < \cdots < \lambda_6\) are the eigenvalues of the Laplacian \(\mathcal{L}\) of \(G\). Moreover, \(\kappa(G) = 13/3 + (2/3)\sqrt{12}\). Then the bounds given in Theorem 2 are approximately: \(3.232 \leq \chi(G) \leq 3.41\). The actual value of \(\chi(G)\) is \(6/\sqrt{12} + 3/2 \approx 3.232\). In fact, \(\chi(G) = (1/2)[7 - (3/2)(7 - \kappa(G))]\).

The graph \(G^{(2)}\) is a complete graph with 7 vertices, the corresponding valuation is \(w^{(2)}(i,j) = 1/\sqrt{6}\) if \(i \neq j\), \(w^{(2)}(i,j) = 1/\sqrt{2}\) if \(i = j\).

A simple calculation shows \(\chi(G^{(5)}, w^{(2)}) \approx 2.6\). Then by (2) of Section 2, \(\chi(G^{(5)}, w^{(2)}) \leq (5/\sqrt{6})\chi(G^{(2)}, w^{(2)}) \approx 5.307\). In fact, \(\chi(G^{(5)}) = 21/2\sqrt{6} \approx 4.28\). The bound given by Theorem 1 is not as good. In fact,
The graph $G^{(3)}$ is depicted in Fig. 1(b). For an edge $i - j$ with $i \neq j$ we have $w^{(3)}(i, j) = 1/2\sqrt{3}$; moreover, $w^{(3)}(i, i) = 1/\sqrt{3}$ if $i \neq 7$ and $w^{(3)}(7, 7) = 3$. It is straightforward to compute the corresponding bounds.

(5) Some authors prefer to consider higher connectivity indices defined in the following way:

$$m_{z}(G) = \frac{1}{\sum_{i_1 - i_2 \cdots - i_{m+1}} \sqrt{d_{i_1}d_{i_2} \cdots d_{i_{m+1}}}},$$

where $i_1 - i_2 \cdots - i_{m+1}$ runs over all paths without repeated vertices. With the obvious modifications of the above results we get the following proposition.

**Proposition.** Let $G$ be a simple graph with vertices $1, \ldots, n$. Then

$$m_{z}(G) \leq \frac{D^{m-1}}{2n^{(m)}(G)},$$

where $n^{(m)}(G)$ is the number of vertices $i$ of $G$ such that there exists at least one path $i = i_1 - i_2 \cdots - i_{m+1}$ without repeated vertices.

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