ON CLIQUE VERSION OF THE RANDIC INDEX

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Abstract. In this paper, we first review the weighted-version of the handshaking lemma based on the idea of a weighted vertex-edge incidence matrix of a given graph $G$. Then, we obtain a generalized version of the handshaking lemma based on the concept of the clique value. We also define a generalized version of Randić index. More importantly, we prove an upper bound for the generalized Randić index of a graph $G$. We finally conclude the paper with some discussions about possible future works.

1. Introduction and Motivation

One of the important parameters of a simple, finite graph is the degree of a vertex. It simply reflects a topological property of a graph which is the size of an open neighborhood of a given vertex. Therefore, one interesting line of research in graph theory is to generalize this local concept and also seeking for its potential applications.

In [1], the author of this paper has suggested an extension this concept to the value of an edge $e = \{u,v\}$ as the size of the intersection of the open neighborhoods of its end-vertices; that is \(\text{val}_G(e) = |N_G(u) \cap N_G(v)|\). He also has used this idea in [1] to find a new upper bound for the number of edges with respect to the number of triangles in any $K_4$-free graph.

The well-known Randić index $R(G)$ of a graph $G$ was introduced in 1975 by Randić [2]. More precisely, he has defined it by

\[
R(G) := \sum_{\{u,v\} \in E(G)} \frac{1}{\sqrt{\text{deg}_G(u) \text{deg}_G(v)}}.
\]

Indeed, in this paper we will call it the vertex-version of Randić index. It seems that this parameter is very useful in mathematical chemistry and has been extensively investigated in the literature (see [3] and the references therein). It is worth to mention the following two classical results in the context of Randić index.

**Theorem 1.1** (Bollobas and Erdos [4]). For any connected graph $G$ with $n$ vertices, $R(G) \geq \sqrt{n-1}$ with equality if and only if $G \cong K_{1,n-1}$.

**Theorem 1.2** (Fajtlowicz [5]). For a graph $G$ with $n$ vertices, $R(G) \leq \frac{n}{2}$ with equality if and only if each component of $G$ has all least two vertices and is regular.
Our main goal in this paper is to obtain an extension of Theorem 1.2, based on the idea of the value of a clique.

2. Basic Definitions and Notations

We assume that our graphs are simple, finite and undirected. For a given graph \( G = (V, E) \) and a vertex \( v \in V(G) \), the set of vertices adjacent to \( v \) is called the open neighborhood of \( v \) in \( G \) and will be denoted by \( N_G(v) \).

The cardinality of \( N_G(v) \) is called the degree of \( v \) and is denoted by \( \deg_G(v) \). A complete subgraph of \( G \) is called a clique of \( G \). A clique on \( k \) vertices is called a \( k \)-clique. A clique on 3 vertices is called a triangle. We will denote the set of triangles of \( G \) by \( T(G) \). We denote the set of all \( k \)-cliques of \( G \) by \( \Delta_k(G) \). The number of \( k \)-cliques of \( G \) is denoted by \( c_k(G) \). We also recall that the well-known Cauchy-Schwartz is the following inequality.

Lemma 2.1. \( \text{[Geometric-Harmonic Mean Inequality]} \) For any real sequences \( \{a_k\}_{k \geq 1} \), we have

\[
\sqrt[k]{a_1a_2\cdots a_k} \geq \frac{k}{\frac{1}{a_1} + \frac{1}{a_2} + \cdots + \frac{1}{a_k}},
\]

with equality whenever \( a_1 = a_2 = \cdots = a_k \).

In what follows, we quickly review the weighted-version of the well-known handshaking lemma and one of its consequences which is known as Mantel’s theorem for triangle-free graphs.

The weighted-version of the well-known handshaking lemma can be read, as follows. From now on, we will denote the set of non-negative real numbers with \( \mathbb{R}^+ \).

Lemma 2.2 (Weighted Handshaking Lemma \[6\]). Let \( G = (V, E) \) be a graph and \( f : V(G) \mapsto \mathbb{R}^+ \) be a non-negative weight function. Then, we have

\[
\sum_{v \in V(G)} f(v) \deg_G(v) = \sum_{e = uv \in E(G)} \left( f(u) + f(v) \right).
\]

In particular, we have

\[
\sum_{v \in V(G)} \deg^2_G(v) = \sum_{e = uv \in E(G)} \left( \deg_G(u) + \deg_G(v) \right).
\]

3. A vertex-version of Randic index

In chemical graph theory literature, the branching index of a given graph \( G \) is known as the Randić index of the graph \( G \) denoted by \( R(G) \). Here, we
will denote it by $R_v(G)$ and call it *vertex-version Randić index* of $G$. It is defined, as follows

\[(3.1) \quad R_v(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}}.\]

In [6], the following result is proved by a simple argument based on the *weighted version of handshaking* lemma and *geometric-harmonic mean* inequality.

**Theorem 3.1** ([5]). For a graph $G$ of order $n$,

\[R_v(G) \leq \frac{n}{2},\]

with equality if and only if every component of $G$ is regular and $G$ has no isolated vertices.

For the sake of completeness, here we also provide a short proof of Theorem 3.1 based on the reference [6].

**Proof.** First, we note that by defining the function $f$ in the equation (2.2) by

\[(f(v) = \begin{cases} \frac{1}{\deg_G(v)} & \text{if } \deg_G(v) > 0, \\ 1 & \text{if } \deg_G(v) = 0, \end{cases}\]

we obtain

\[(3.2) \quad \sum_{uv \in E(G)} \left( \frac{1}{\deg_G(u)} + \frac{1}{\deg_G(v)} \right) = n - n_0,\]

where $n_0$ denotes the number of isolated vertices in $G$. Now considering the *geometric-harmonic* inequality for $k = 2$, Lemma 2.1, we have

\[(3.3) \quad R_v(G) \leq \sum_{e=uv \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}} \leq \sum_{uv \in E(G)} \frac{1}{2} \left( \frac{1}{\deg_G(u)} + \frac{1}{\deg_G(v)} \right) = \frac{n - n_0}{2} \leq \frac{n}{2},\]

as required. \[\square\]
4. AN EDGE-VERSION OF RANDIC INDEX

In this section, we aim to obtain an edge version of the upper bound for the Randić index, based on the new concept of the value of an edge.

**Definition 4.1.** Let $G = (V, E)$ be a graph and $e = uv$ be an edge of $G$. Then, we define the edge value of $e$, denoted by $val_G(e)$, as follows

$$\text{(4.1)} \quad val_G(e) = |N_G(e)| = |N_G(u) \cap N_G(v)|.$$ 

Here, $N_G(e)$ denotes the set of common neighbors of end vertices of the edge $e$.

Next, we generalize the weighted handshaking lemma for values of edges of a given graph.

**Lemma 4.1.** [Weighted Edge Handshaking Lemma] Let $G = (V, E)$ be a graph and $g : E(G) \mapsto \mathbb{R}^+$ be a non-negative weight function. Then, we have

$$\text{(4.2)} \quad \sum_{e \in E(G)} g(e) val_G(e) = \sum_{\delta = e_1 e_2 e_3 \in T(G)} \left( g(e_1) + g(e_2) + g(e_3) \right).$$

In particular, we have

$$\text{(4.3)} \quad \sum_{e \in E(G)} \text{val}_G^2(e) = \sum_{\delta = e_1 e_2 e_3 \in T(G)} \left( \text{val}_G(e_1) + \text{val}_G(e_2) + \text{val}_G(e_3) \right).$$

As an immediate consequence of the above lemma, we have the following interesting result. Recall that an edge $e \in E(G)$ is called isolated if we have $val_G(e) = 0$.

**Corollary 4.2.** For any graph $G$ with $m$ edges, we have

$$\text{(4.4)} \quad \sum_{\delta = e_1 e_2 e_3 \in T(G)} \left( \frac{1}{\text{val}_G(e_1)} + \frac{1}{\text{val}_G(e_2)} + \frac{1}{\text{val}_G(e_3)} \right) = m - m_0,$$

in which $m_0$ is the number of isolated edges.

Next, we give a generalization of the result in [5]. To do so, we first need to give a generalization of the concept of Randić index.

**Definition 4.2.** For a given graph $G = (V, E)$, the edge-version of the Randić index, denoted by $R_e(G)$, is defined as

$$\text{(4.5)} \quad R_e(G) := \sum_{\delta = e_1 e_2 e_3 \in T(G)} \frac{1}{\text{val}_G(e_1) \text{val}_G(e_2) \text{val}_G(e_3)}.$$ 

From now on, we will call a graph edge-regular if $val_G(e)$ is the same for all edges of $G$. 
**Theorem 4.3.** For a graph $G$ of size $m$, we have

$$R_e(G) \leq \frac{m}{3},$$

with equality if and only if every component of $G$ is edge-regular and $G$ has no isolated edges.

**Proof.** Considering Corollary 4.2 and arithmetic-geometric inequality, we have

$$R_e(G) := \sum_{\delta = e_1 e_2 e_3 \in T(G)} \frac{1}{\sqrt{\text{val}_G(e_1) \text{val}_G(e_2) \text{val}_G(e_3)}}$$

$$\leq \frac{1}{3} \sum_{\delta = e_1 e_2 e_3 \in T(G)} \left( \frac{1}{\text{val}_G(e_1)} + \frac{1}{\text{val}_G(e_2)} + \frac{1}{\text{val}_G(e_3)} \right)$$

$$= \frac{1}{3} (m - m_0) \leq \frac{m}{3}. \quad \square$$

5. **THE CLIQUE HANDSHAKING LEMMA**

In this section, we attempt to find a more generalized version of Randić index which we call it the generalized Randić index. To this end, we first need to present an extension of the definition of the degree of vertex to the value of any clique of higher order.

**Definition 5.1.** Let $G = (V, E)$ be a graph and $q_k \in \Delta_k(G)$ be a $k$-clique in $G$. Then, we define the value of the clique $q_k$ with the vertex set $V(q_k) = v_{i_1} \cdots v_{i_k}$ denoted by $\text{val}_G(q_k)$, as follows

$$\text{val}_G(q) = \left| \bigcap_{i=1}^{k} N_G(v_{i_i}) \right|.$$  

We will also call an $k$-clique $q_k$ with $\text{val}_G(q_k) = 0$, an isolated clique of $G$.

Note that any $k$-clique $q_k = v_{i_1} \cdots v_{i_k} \in \Delta_k(G)$ in $G$ can also be represented (uniquely) by $q_k = q_{k-1,1} \cdots q_{k-1,k}$ where for each $i = 1, \ldots, k$ the symbol $q_{k-1,i}$ denotes a $(k-1)$-clique subgraph of $q_k$. We will use this fact in our next key lemma.

**Lemma 5.1 (Weighted Clique Handshaking Lemma).** Let $G = (V, E)$ be a graph and and let $h : \Delta_k(G) \mapsto \mathbb{R}^+ \ (k \geq 2)$ be a weight function. Then, we have

$$\sum_{q_k \in \Delta_k(G)} h(q_k) \text{val}_G(q_k) = \sum_{q_{k+1} = q_{k,1} \cdots q_{k,k+1} \in \Delta_{k+1}(G)} \left( h(q_{k,1}) + \ldots + h(q_{k,k+1}) \right).$$

In particular, we have
(5.3) \[ \sum_{q_k \in \Delta_k(G)} \text{val}_G^2(q_k) = \sum_{q_{k+1} = q_{k,1} \cdots q_{k,k+1} \in \Delta_{k+1}(G)} \left( \text{val}_G(q_{k,1}) + \cdots + \text{val}_G(q_{k,k+1}) \right). \]

Proof. We proceed by defining the weighted subclique-superclique matrix \( I_{f,k}(G) \) of order \( k \), as follows

\[
(I_{f,k}(G))_{q_k,q_{k+1}} = \begin{cases} h(q_k) & \text{if } q_k \text{ is a subgraph of } q_{k+1}, \\ 0 & \text{otherwise}. \end{cases}
\]

Next, we note that in the matrix \( I_{f,k}(G) \) each row corresponding to the clique \( q_k \) has \( \text{val}_G(q_k) \) non-zero entries. Hence, the resulting row-sum equals \( h(q_k) \text{val}_G(q_k) \). On the other hand, each column corresponding to the clique \( q_{k+1} = q_{k,1} \cdots q_{k,k+1} \) has the column-sum \( h(q_{k,1}) + \cdots + h(q_{k,k+1}) \). Thus, by summing over all rows and columns and equating them we get the desired result.

□

6. The Generalized Randić Index

In this last section, we obtain a more generalized version of Randić index which we call it the generalized Randić index.

Next, we define the generalized Randić index of a graph \( G \) or a clique-version of the Randić index based on the new concept of the clique value in graph theory.

**Definition 6.1.** Let \( G = (V, E) \) be a graph. Then, the generalized Randić index of \( G \), denoted by \( R_{c_{\text{clq}}}(G) \), is defined by

\[
R_{c_{\text{clq}}}(G; k) := \sum_{q_{k+1} = q_{k,1} \cdots q_{k,k+1} \in \Delta_{k+1}(G)} \frac{1}{\prod_{j=1}^{k+1} \text{val}_G(q_{k,j})}, \quad (k \geq 1)
\]

We first need the following key result.

**Proposition 6.1.** Let \( G = (V, E) \) be a graph. Then, we have

\[
\sum_{q_{k+1} = q_{k,1} \cdots q_{k,k+1} \in \Delta_{k+1}} \left( \frac{1}{\text{val}_G(q_{k,1})} + \cdots + \frac{1}{\text{val}_G(q_{k,k+1})} \right) = c_k(G) - c_{k,0}(G),
\]

in which \( c_{k,0}(G) \) is the number of isolated \( k \)-cliques of \( G \).

Now, we are at the position to state the main result of this paper which a generalized version of the result in [5]. Form now one, a graph in which all values of \( \text{val}_G(q_k) \) are the same for \( k \)-cliques of \( G \) is called \( k \)-clique regular graph.
Theorem 6.2. Let $G$ be a graph. Then, we have

$$R_{clq}(G; k) \leq \frac{c_k(G)}{k + 1}.$$ 

The equality holds if and only if each component of $G$ is a $k$-clique regular graphs.

Proof. The proof is straight forward based on Proposition 6.1 and the arithmetic-geometric mean inequality.

□

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