



The generalized Randić Index of Graphs

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Abstract

In this paper, we first review the weighted-version of the handshaking lemma based on the weighted-version of the incidence matrix of a given graph G . Then, we obtain an extension of the handshaking lemma based on the new concept of the value of a clique in G . We also define a clique version of the Randić index that we will call it the generalized Randić index. More importantly, we obtain a generalization of the well-know upper bound for the Randić index of a graph G due to Fajtlowicz. We finally conclude the paper with some discussions about possible future works.

Keywords: The value of an edge, The value of a clique, The clique handshaking lemma.

2020 MSC: 05C50, 65H04.

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1. Introduction

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

In [4], the author of this paper has introduced an extension this concept to the value of an edge $e = \{u, v\}$ as the number of common neighborhoods of its end-vertices, that is $\text{val}_G(e) = |N_G(u) \cap N_G(v)|$. He also has applied this new idea in [4] to find a new upper bound for the number of edges with respect to the number of triangles in K_4 -free graphs.

The well-known Randić index $R(G)$ of a graph G was introduced in 1975 by Randić [3]. More precisely, he defined this index by

$$R(G) := \sum_{\{u,v\} \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}}. \quad (1.1)$$

The Randić index is very useful in mathematical chemistry and has been extensively investigated in the literature (see [3] and the references therein). Next, we mention the following two important classical results in the context of the Randić index.

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Received: January 10, 2023 Revised: January 23, 2023 Accepted: January 28, 2023

Theorem 1.1 (Bollobás and Erdős [1]). 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 [2]). For a graph G with n vertices, $R(G) \leq \frac{n}{2}$ with equality if and only if each component of G has at least two vertices and is regular.

Our main goal here is to obtain a generalization of Theorem 1.2, based on the idea of the value of a clique in a given graph.

2. Basic Definitions and Notations

Throughout this paper, we will assume that our graphs are simple, finite and undirected. For a given graph $G = (V, E)$ and a vertex $v \in V(G)$, the open neighborhood of v , denoted by $N_G(v)$, is the set of vertices adjacent to v . The cardinality of $N_G(v)$ is called the degree of the vertex of v and is denoted by $\deg_G(v)$. A complete subgraph of G is the one in which each pair of vertices are connected. We will also call it a clique of G . A clique with k vertices is called a k -clique. A clique on 3 vertices is called a triangle. The set of triangles of G is denoted by $T(G)$. We denote the set of all k -cliques of G by $\Delta_k(G)$. We also denote the number of k -cliques of G by $c_k(G)$. We also recall the well-known geometric-harmonic mean inequality, as follows.

Lemma 2.1. [Geometric-Harmonic Mean Inequality] For any sequence $\{a_k\}_{k \geq 1}$ of positive real numbers, we have

$$\sqrt[k]{a_1 a_2 \cdots a_k} \geq \frac{k}{\frac{1}{a_1} + \frac{1}{a_2} + \cdots + \frac{1}{a_k}}, \tag{2.1}$$

with equality whenever $a_1 = a_2 = \cdots = a_k$.

Next, we quickly review the basics of the weighted-version of the well-known handshaking lemma. The weighted-version of the well-known handshaking lemma can be read, as follows. The proof is straight forward and based on the double counting technique. From now on, we will denote the set of non-negative real numbers with \mathbb{R}^+ .

Lemma 2.2 (Weighted Handshaking Lemma [5]). Let $G = (V, E)$ be a graph and $f : V(G) \mapsto \mathbb{R}^+$ be a non-negative weight function. Then, we have

$$\sum_{v \in V(G)} f(v) \deg_G(v) = \sum_{e=uv \in E(G)} (f(u) + f(v)). \tag{2.2}$$

In particular, we have

$$\sum_{v \in V(G)} \deg_G^2(v) = \sum_{e=uv \in E(G)} (\deg_G(u) + \deg_G(v)). \tag{2.3}$$

We note that one of the interesting consequences of the equation (2.3) is the following.

Theorem 2.3 (Mantel’s theorem for K_3 -free graphs). Let $G = (V, E)$ be a triangle-free graph. Then, we have

$$|E(G)| \leq \frac{|V(G)|^2}{4}. \tag{2.4}$$

3. The vertex-version of the Randić index

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

$$R_V(G) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}}. \tag{3.1}$$

In [5], the following result is proved by a simple argument based on the weighted version of the hand-shaking lemma and the geometric-harmonic mean inequality.

Theorem 3.1 ([2]). 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 [5].

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

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

we obtain

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

where n_0 denotes the number of isolated vertices in G .

Now by considering geometric-harmonic inequality for $k = 2$, Lemma 2.1, we get

$$\begin{aligned} R_V(G) &= \sum_{e=uv \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}} \leq \sum_{uv \in E(G)} \frac{1}{2} \left(\frac{1}{\deg_G(u)} + \frac{1}{\deg_G(v)} \right) \\ &= \frac{n - n_0}{2} \leq \frac{n}{2}, \end{aligned}$$

as required. □

4. The edge-version of Randić index

In this section, we aim to obtain an edge-version of the classical Randić index based on a generalization of the concept of the degree of a vertex.

Definition 4.1. Let $G = (V, E)$ be a graph and $e = \{u, v\}$ be an edge of G . Then, we define the value of an edge e , denoted by $\text{val}_G(e)$, as follows

$$\text{val}_G(e) = |N_G(e)| = |N_G(u) \cap N_G(v)|. \tag{4.1}$$

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

Next, using a double-counting technique, we can generalize the weighted handshaking lemma for values of edges of a given graph.

Lemma 4.2 (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

$$\sum_{e \in E(G)} g(e) \text{val}_G(e) = \sum_{\delta = e_1 e_2 e_3 \in T(G)} (g(e_1) + g(e_2) + g(e_3)). \tag{4.2}$$

In particular, we have

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

As an immediate consequence of the above lemma, we have the following interesting result. Recall that an edge $e \in E(G)$ is said to be isolated, if we have $\text{val}_G(e) = 0$.

Corollary 4.3. For any graph G with m edges, we have

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

in which m_0 is the number of isolated edges.

Next, we give a generalization of the result in [2]. To do so, we first need to give a generalization of the concept of the vertex-version of the Randić index. From now on, a graph in which the values of its edges are the same is called the edge-regular graph.

Definition 4.4. For a given graph $G = (V, E)$, the edge-version of the Randić index, denoted by $R_E(G)$, is defined as

$$R_E(G) := \sum_{\delta = e_1 e_2 e_3 \in T(G)} \frac{1}{\sqrt{\text{val}_G(e_1) \text{val}_G(e_2) \text{val}_G(e_3)}}, \tag{4.5}$$

where the sum runs over all triangles of G .

Theorem 4.5. For a graph G with m edges, we have

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

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

Proof. Considering Corollary 4.3 and the geometric-harmonic mean inequality 2.1 (for $k = 3$), we have

$$\begin{aligned} R_E(G) &:= \sum_{\delta = e_1 e_2 e_3 \in T(G)} \frac{1}{\sqrt{\text{val}_G(e_1) \text{val}_G(e_2) \text{val}_G(e_3)}} & (4.6) \\ &\leq \frac{1}{3} \sum_{\delta = e_1 e_2 e_3 \in T(G)} \left(\frac{1}{\text{val}_G(e_1)} + \frac{1}{\text{val}_G(e_2)} + \frac{1}{\text{val}_G(e_3)} \right) \\ &= \frac{1}{3} (m - m_0) \leq \frac{m}{3}. \end{aligned}$$

□

5. A clique-version of Randić Index

In this section, we first attempt to find a more generalized version of handshaking lemma. Then, we present the main result of the paper which is a clique-version of Theorem 3.1.

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 $V(q_k) = \{v_{i_1}, \dots, v_{i_k}\}$ denoted by $\text{val}_G(q_k)$, as follows

$$\text{val}_G(q_k) = \left| \bigcap_{v \in V(q_k)} N_G(v) \right|. \tag{5.1}$$

We also mention that any k -clique q_k with $\text{val}_G(q_k) = 0$ is called an isolated k -clique. Moreover, a graph in which all k -cliques have the same value is called an k -clique regular graph.

Remark 5.2. Note that any k -clique $q_k \in \Delta_k(G)$ in G can also be represented (uniquely) by $q_k = q_{k-1,1} \cdots q_{k-1,k}$ where for each $i = 1, \dots, k$ 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 5.3 (Weighted Clique Handshaking Lemma [4]). Let $G = (V, E)$ be a graph and let $h : \Delta_k(G) \mapsto \mathbb{R}^+$ ($k \geq 1$) be a non-negative weight function. Then, we have

$$\sum_{q_k \in \Delta_k(G)} h(q_k) \text{val}_G(q_k) = \sum_{q_{k+1} = q_{k,1} \cdots q_{k,k+1} \in \Delta_{k+1}(G)} \left(h(q_{k,1}) + \cdots + h(q_{k,k+1}) \right). \tag{5.2}$$

In particular, we have

$$\sum_{q_k \in \Delta_k(G)} \text{val}_G^2(q_k) = \sum_{q_{k+1} = q_{k,1} \cdots q_{k,k+1} \in \Delta_{k+1}(G)} \left(\text{val}_G(q_{k,1}) + \cdots + \text{val}_G(q_{k,k+1}) \right). \tag{5.3}$$

Proof. We proceed by defining the weighted subclique-superclique incidence matrix $I_{f,k}(G)$ of order $|\Delta_k(G) \times \Delta_{k+1}(G)|$, 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 to $h(q_k) \text{val}_G(q_k)$. 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. □

We note that in the special case of $k = 1$, the matrix $I_{f,1}(G)$ is exactly the standard vertex-edge incidence matrix of a graph G .

6. The Generalized Randić Index

In this section, we find a more generalized version of Theorem 3.1 based on the idea of the weighted clique handshaking lemma.

We first define the generalized Randić index of a graph G or a cliuqe-version of Randić index based on the new concept of the value of a clique in graph theory.

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

$$R_{\text{cliq}}(G; k) := \sum_{q_{k+1}=q_{k,1}\cdots q_{k,k+1} \in \Delta_{k+1}(G)} \frac{1}{\sqrt{\prod_{j=1}^{k+1} \text{val}_G(q_{k,j})}}, \quad (k \geq 1), \quad (6.1)$$

where the sum runs over all $(k+1)$ -cliques of G .

We then need the following key result, as an extension of Corollary 4.3.

Proposition 6.2. Let $G = (V, E)$ be a graph. Then, we have

$$\sum_{q_{k+1}=q_{k,1}\cdots q_{k,k+1} \in \Delta_{k+1}} \left(\frac{1}{\text{val}_G(q_{k,1})} + \cdots + \frac{1}{\text{val}_G(q_{k,k+1})} \right) = c_k(G) - c_{k,0}(G), \quad (6.2)$$

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 [2].

Theorem 6.3. Let G be a graph. Then, we have

$$R_{\text{cliq}}(G; k) \leq \frac{1}{k+1} c_k(G), \quad (6.3)$$

and the equality holds if and only if each component of G is k -clique regular and G has no isolated k -cliques.

Proof. The proof is straight forward considering Proposition 6.2 and the geometric-harmonic inequality (Lemma 2.1). □

7. Concluding Remarks

In this paper, we first introduced an edge-version of the well-known Randić index of a finite, simple and undirected graph G by extending the definition of the concept of the degree of a vertex to the degree (or value) of an edge (a pair of connected vertices). The key ingredient of the proof was a weighted form of an edge-version of the handshaking lemma. Then, we introduce an even more generalized version of the Randić index the so called generalized Randić index by presenting a higher order analogue of the concept of the degree of a vertex as the value of any higher order k -clique ($k > 1$). The main idea was based on a weighted-version of the clique handshaking lemma. The next step of our research project is to study a clique-version of the general Randić index $R_\alpha(G)$, defined by

$$R_\alpha(G) = \sum_{e=uv \in E(G)} (\deg_G(u) \deg_G(v))^\alpha,$$

where α is a real number in the interval $(0, 1)$.

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