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Local Value of a Vertex-Degree Function Index of a Graph

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Abstract

Let n be a positive integer and f a real function defined on integers in the interval $[1, n-1]$. Given a graph G with vertex set V and n non-isolated vertices, the degree-function index of G is defined as $H_f(G) = \sum_{u \in V} f(d_u)$. It is our main objective in this paper to introduce the local value of a degree-function index H_f of a graph G at a vertex u, which we denote by $f_G(u)$. Intutively, $f_G(u)$ measures the contribution of vertex u in $H_f(G)$. In this paper we initiate the study of its mathematical properties and address the problem of vertices with extremal local values in the zeroth-order general Randić index. In particular, for the first Zagreb index and the forgotten index, the problem of vertices with extremal local values is completely solved.

1 Introduction

Let G be a simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. We denote by $d_G(u)$ the degree of the vertex $u \in V$. If it is clear from the context, we simply write $d_u = d_G(u)$. The set $\mathcal{N}_G(u)$ denotes the set of neighbors of vertex $u \in V$.

Let n be a positive integer and let $f : [1, n-1] \cap \mathbb{N} \to \mathbb{R}$ be a real function. Instead of using H_f, we use the same letter f to denote the vertex-degree function index $f : \mathcal{G}_n \to \mathbb{R}$ as

$$f(G) = \sum_{v \in V(G)} f(d_v), \tag{1}$$

where $\mathcal{G}_n$ is the set of all graphs with n vertices and $G \in \mathcal{G}_n$. This concept was originally introduced by N. Linial and E. Rozenman in 2002 [9], and recently there has been intensive research activity in this direction, as we can see in the papers [2, 3, 10–13], just to mention a few.

One significative type of vertex-degree function indices were introduced by Li and Zheng in 2005 [8], the so called zeroth-order general Randić index, induced by the function $\mathcal{R}_\alpha : [1, n-1] \cap \mathbb{N} \to \mathbb{R}$ defined as $\mathcal{R}_\alpha(x) = x^\alpha$, where $\alpha \in \mathbb{R}$. So given a graph G with n non-isolated vertices,

$$\mathcal{R}_\alpha(G) = \sum_{u \in V(G)} \mathcal{R}_\alpha(d_u) = \sum_{u \in V(G)} (d_u)^\alpha .$$

Particularly important is the case $\alpha = 2$, which corresponds to the first Zagreb index [6]

$$\mathcal{R}_2(G) = \sum_{u \in V} d_u^2 = \sum_{vw \in E} (d_v + d_w),$$

and the case $\alpha = 3$, which was called by Furtula and Gutman [5] the forgotten index, but first appeared in [6],

$$\mathcal{R}_3(G) = \sum_{u \in V} d_u^3 = \sum_{vw \in E} \left(d_v^2 + d_w^2\right).$$

In recent papers [1, 4], the concept of local energy at a vertex was introduced with the intention to give a measure of the contribution of a vertex in the total energy of the graph. Our main objective in this paper is to introduce the local value of a degree-function index f at a vertex u of a graph G, which we will denote by $f_G(u)$. Intuitively, $f_G(u)$ is the contribution of the vertex u in $f(G)$. Moreover, the definition of local value of a degree-function index at a vertex is such that the following formula holds:

$$\sum_{u \in V} f_G(u) = f(G).$$

In Section 2 we compute the local values of a degree-function index in well-known graphs, and then we initiate the study of its mathematical properties. Later, in Section 3, we address the problem of vertices with extremal values in the zeroth-order general Randić index. In the particular cases of the first Zagreb index and the forgotten index, the problem of vertices with extremal local values is completely solved.

2 Local value of a vertex-degree function index of a graph

Throughout this paper, n is a positive integer and $f : [1, n-1] \cap \mathbb{N} \to \mathbb{R}$ is a function. Given a graph G with n non-isolated vertices, clearly $d_G(u) \in [1, n-1] \cap \mathbb{N}$ for all $u \in V(G)$, so that $f(G) = \sum_{u \in V} f(d_u)$ is well defined in (1).

Definition 1. Let G be a graph with n non-isolated vertices. We define the local value of f at $u \in V(G)$, denoted by $f_G(u)$, as

$$f_G(u) = (1 - d_u) f(d_u) + \sum_{w \in \mathcal{N}(u)} f(d_w). \tag{2}$$

The value $f_G(u)$ can be interpreted as the contribution of vertex u in $f(G)$.

Example 1. Let S_n be the star tree with n vertices. We can easily compute $f_{S_n}(u)$, for any vertex $u \in V(S_n)$. There are two possibilities:

1. If u is the center vertex of S_n, then

$$\begin{aligned} f_{S_n}(u) &= [1 - (n-1)] f(n-1) + (n-1) f(1) \\ &= (2-n) f(n-1) + (n-1) f(1). \end{aligned}$$

2. If v is a pendent vertex of S_n, then

$$f_{S_n}(v) = (1-1) f(1) + f(n-1) = f(n-1).$$

Note that in the previous example

$$\sum_{w \in V(S_n)} f_{S_n}(w) = f_{S_n}(u) + (n-1) f_{S_n}(v) = f(S_n).$$

We next show that this is true for all graphs. First we need a preliminary result.

Lemma 1. *Let G be a graph with n non-isolated vertices. Then,*

$$\sum_{u \in V(G)} \sum_{w \in \mathcal{N}_G(u)} f(d_w) = \sum_{u \in V(G)} d_u f(d_u). \tag{3}$$

Proof. For each $u \in V(G)$, the term $f(d_u)$ appears d_u times in the sum on the left side of (3). ■

Theorem 1. *Let G be a graph with n non-isolated vertices. Then,*

$$\sum_{u \in V(G)} f_G(u) = f(G).$$

Proof. Let $u \in V(G)$. Then by (2)

$$f_G(u) = f(d_u) - d_u f(d_u) + \sum_{w \in \mathcal{N}_G(u)} f(d_w). \tag{4}$$

Now taking sums on both sides of (4) over all $u \in V(G)$, and using Lemma 1, we deduce

$$\begin{aligned}\sum_{u \in V(G)} f_G(u) &= f(G) - \sum_{u \in V(G)} d_u f(d_u) + \sum_{u \in V(G)} \sum_{w \in \mathcal{N}_G(u)} f(d_w) && (5)\\ &= f(G) - \sum_{u \in V(G)} d_u f(d_u) + \sum_{u \in V(G)} d_u f(d_u) && (6)\\ &= f(G).\end{aligned}$$

■

Example 2. Let us consider some examples of local values of a vertex-degree function index of well known graphs.

1. Let K_n be the complete graph with n vertices. Then for any $u \in V(K_n)$,

$$f_{K_n}(u) = (1 - (n-1)) f(n-1) + (n-1) f(n-1) = f(n-1).$$

2. Let C_n be the cycle with n vertices. Then for any $u \in V(C_n)$,

$$f_{C_n}(u) = (1-2) f(2) + 2f(2) = f(2).$$

3. Let P_n be the path with n vertices. If v_1 is a pendent vertex of P_n, then

$$f_{P_n}(v_1) = (1-1) f(1) + f(2) = f(2).$$

   If v_2 is a vertex of P_n adjacent to a pendent vertex, then

$$f_{P_n}(v_2) = (1-2) f(2) + f(1) + f(2) = f(1).$$

   Finally, if v_3 is a vertex of P_n with both neighbors of degree 2, then

$$f_{P_n}(v_3) = (1-2) f(2) + f(2) + f(2) = f(2).$$

4. Let $K_{p,q}$ the complete bipartite graph. If $u \in V(K_{p,q})$ is such that $d_{K_{p,q}}(u) = q$, then

$$\begin{aligned} f_{K_{p,q}}(u) &= (1-q) f(q) + qf(p) \\ &= f(q) + q[f(p) - f(q)]. \end{aligned}$$

   Similarly, if $v \in V(K_{p,q})$ is such that $d_{K_{p,q}}(v) = p$, then

$$\begin{aligned} f_{K_{p,q}}(v) &= (1-p) f(p) + pf(q) \\ &= f(p) + p[f(q) - f(p)]. \end{aligned}$$

Note that the local value of f in K_n and C_n is constant for all vertices. More generally, we have the following result.

Proposition 2. *Let G be a regular graph of degree k. Then for any $u \in V(G)$,*

$$f_G(u) = f(k).$$

Proof. Let $u \in V(G)$. Then

$$f_G(u) = (1-k) f(k) + \sum_{w \in \mathcal{N}_G(u)} f(d_w) = (1-k) f(k) + k f(k) = f(k).$$

■

The converse of Proposition 2 does not hold.

Example 3. Consider the vertex-degree function index induced by $f(x) = x^2 - 3x$. Note that $f(1) = f(2) = -2$. Hence, every vertex in P_n has constant local value -2 (see Example 2).

When computing the local value of a vertex-degree function index f at a vertex u in a graph G, we can restrict our attention to the component of G which contains the vertex u.

Proposition 3. *Let $G = H \cup K$ be the disjoint union of graphs H and K. Let $u \in V(H)$. Then $f_G(u) = f_H(u)$.*

Proof. Clearly, $d_G(u) = d_H(u)$ and $d_G(w) = d_H(w)$, for all $w \in \mathcal{N}_G(u) = \mathcal{N}_H(u)$. Hence

$$\begin{aligned} f_G(u) &= (1 - d_G(u)) f(d_G(u)) + \sum_{w \in \mathcal{N}_G(u)} f(d_G(w)) \\ &= (1 - d_H(u)) f(d_H(u)) + \sum_{w \in \mathcal{N}_H(u)} f(d_H(w)) \\ &= f_H(u). \end{aligned}$$

■

Several questions arise when considering the local value of a vertex-degree function index f at a vertex u in a graph G:

1. If H is an induced subgraph of a graph G and $u \in V(H)$, is there a relation between $f_G(u)$ and $f_H(u)$?

2. Let $u \in V(G)$. If $v \in V(G)$ is such that $d_v > d_u$, is there a relation between $f_G(u)$ and $f_G(v)$?

Example 4. Let us consider the forgotten index induced by the function $\mathcal{R}_3(x) = x^3$, and let H be the induced subgraph of $K_{3,3}$ shown in Figure 1. Then,

$$(\mathcal{R}_3)_{K_{3,3}}(v_1) = (\mathcal{R}_3)_{K_{3,3}}(v_5) = -2\mathcal{R}_3(3) + 3\mathcal{R}_3(3) = \mathcal{R}_3(3) = 27.$$

However, the local value at v_1 increases:

$$(\mathcal{R}_3)_H(v_1) = (1-2)\mathcal{R}_3(2) + 2\mathcal{R}_3(3) = 46,$$

while the value at v_5 decreases:

$$(\mathcal{R}_3)_H(v_5) = (1-3)\mathcal{R}_3(3) + \mathcal{R}_3(2) + 2\mathcal{R}_3(3) = 8.$$

So in general, if H is a induced subgraph of G and $u \in V(H)$, then $f_H(u)$ can increase or decrease the value of $f_G(u)$.

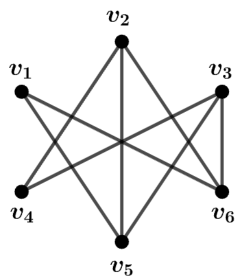

Figure 1. Induced subgraph H of $K_{3,3}$ used in Example 4.

Example 5. Consider the first Zagreb index induced by the function $\mathcal{R}_2(x) = x^2$, and let T be the tree depicted in Figure 2. Note that

$$2 = d_a < d_x = d_y = 3,$$

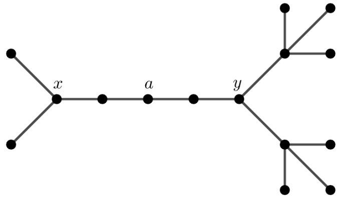

Figure 2. Tree T used in Example 5.

and

$$(\mathcal{R}_2)_T(a) = -\mathcal{R}_2(2) + 2\mathcal{R}_2(2) = 4,$$

$$(\mathcal{R}_2)_T(x) = -2\mathcal{R}_2(3) + 2\mathcal{R}_2(1) + \mathcal{R}_2(2) = -12,$$

$$(\mathcal{R}_2)_T(y) = -2\mathcal{R}_2(3) + \mathcal{R}_2(2) + 2\mathcal{R}_2(4) = 18.$$

Hence, in general, if $u, v \in V(G)$ and $d_v > d_u$, then $f_G(v)$ can increase or decrease the value of $f_G(u)$.

3 Local values of the zeroth-order general Randić index

Let n be a positive number and let $\mathcal{R}_\alpha : [1, n-1] \cap \mathbb{N} \to \mathbb{R}$ be the function defined as $\mathcal{R}_\alpha(x) = x^\alpha$, where $\alpha \in \mathbb{R}$. Given a graph G with n vertices, recall that the function index

$$\mathcal{R}_\alpha(G) = \sum_{u \in V(G)} \mathcal{R}_\alpha(d_u) = \sum_{u \in V(G)} (d_u)^\alpha,$$

is the zeroth-order Randić index of G. In this particular case, the local value of $\mathcal{R}_\alpha$ at $u \in V(G)$ is

$$(\mathcal{R}_\alpha)_G(u) = (1 - d_u)\, d_u^\alpha + \sum_{w \in \mathcal{N}_G(u)} d_w^\alpha.$$

Lemma 2. *The function* $g : [1, n-1] \cap \mathbb{N} \to \mathbb{R}$ *defined as*

$$g(x) = (1-x)\, x^{\alpha} + x \tag{7}$$

is strictly decreasing (resp. strictly increasing) if $\alpha > 0$ *(resp.* $\alpha < 0$*) in* $[1, n-1] \cap \mathbb{N}$*.*

Proof. This can be proved using standard differential calculus. ■

Theorem 4. *Let* G *be a graph with* n *non-isolated vertices,* $u \in V(G)$ *and* $\alpha > 0$*. Then*

$$(\mathcal{R}_{\alpha})_G(u) \geq (2-n)(n-1)^{\alpha} + (n-1). \tag{8}$$

Equality in (8) holds if and only if u *is the center of a star tree with* n *vertices.*

Proof. Since $\alpha > 0$ it is clear that $d_w^{\alpha} \geq 1$ for all $w \in \mathcal{N}_G(u)$. Also, we know from Lemma 2 that g is strictly decreasing on $[1, n-1] \cap \mathbb{N}$, so that $g(d_u) \geq g(n-1)$. Hence

$$\begin{aligned}(\mathcal{R}_{\alpha})_G(u) &= (1-d_u)\, d_u^{\alpha} + \sum_{w \in \mathcal{N}_G(u)} d_w^{\alpha} \\ &\geq (1-d_u)\, d_u^{\alpha} + d_u = g(d_u) \\ &\geq g(n-1) = (2-n)(n-1)^{\alpha} + (n-1). \end{aligned} \tag{9}$$

If u is the center vertex of a star tree with n vertices, then it follows from Example 1 that equality occurs in (8). Conversely, assume that equality in (8) holds. Then by inequality (9), $g(d_u) = g(n-1)$ and $d_w^{\alpha} = 1$, for all $w \in \mathcal{N}_G(u)$. Since g is strictly decreasing, $d_u = n-1$ and $d_w = 1$ for all $w \in \mathcal{N}_G(u)$. Equivalently, G is a star tree with n vertices with center vertex u. ■

Dually we have the following result.

Theorem 5. *Let* G *be a graph with* n *non-isolated vertices,* $u \in V(G)$

and $\alpha < 0$. *Then*

$$\left(\mathcal{R}_{\alpha}\right)_G(u) \leq (2-n)(n-1)^{\alpha} + (n-1). \tag{10}$$

Equality in (10) holds if and only if u *is the center of a star tree with* n *vertices.*

Proof. Similar to the proof of Theorem 4. ■

Given a graph G and a vertex $u \in V(G)$, the problem of finding an upper bound for $\left(\mathcal{R}_{\alpha}\right)_G(u)$ when $\alpha > 0$ is much more complicated. With this objective in mind we begin with a technical result.

Lemma 3. *Let* n *be a positive integer and* $\alpha \geq 1$. *Consider the function* $h : [1, n-1] \cap \mathbb{N} \to \mathbb{R}$ *defined as*

$$h(x) = (1-x)x^{\alpha} + x\left(\frac{n-1}{x}\right)^{\alpha}. \tag{11}$$

Then h *is strictly decreasing in* $[1, n-1] \cap \mathbb{N}$.

Proof. This is an easy application of standard differential calculus. ■

Theorem 6. *Let* G *be a graph with* n *non-isolated vertices,* $u \in V(G)$ *and* $\alpha \geq 1$. *Then*

$$\left(\mathcal{R}_{\alpha}\right)_G(u) \leq (n-1)^{\alpha}. \tag{12}$$

Equality in (12) occurs if and only if u *is a pendent vertex of a star tree with* n *vertices.*

Proof. Let $\mathcal{N}_G(u) = \{w_1, \ldots, w_{d_u}\}$. Set $\sum_{i=1}^{d_u} d_{w_i} = p \leq n-1$. Since $\alpha > 0$, using Lagrange multipliers we deduce that the function $F(x_1, \ldots, x_{d_u}) = \sum_{i=1}^{d_u} x_i^{\alpha}$, subject to the condition $\sum_{i=1}^{d_u} x_i = p$, attains its maximal value at $\left(\frac{p}{d_u}, \frac{p}{d_u}, \ldots, \frac{p}{d_u}\right)$. Consequently, by Lemma 3,

$$\left(\mathcal{R}_{\alpha}\right)_G(u) = (1-d_u)\, d_u^{\alpha} + \sum_{w \in \mathcal{N}_G(u)} d_w^{\alpha}$$

$$\leq (1-d_u)\, d_u^\alpha + d_u \left(\frac{p}{d_u}\right)^\alpha$$

$$\leq (1-d_u)\, d_u^\alpha + d_u \left(\frac{n-1}{d_u}\right)^\alpha$$

$$= h\,(d_u) \leq h\,(1) = (n-1)^\alpha\,. \tag{13}$$

By Example 1, we know that equality holds in (12) when u is a pendent vertex of a star tree with n vertices. Conversely, assume equality holds in (12). Then by inequality (13), $h\,(d_u) = h\,(1)$ (which implies $d_u = 1$ by Lemma 3), $p = n-1$, and $d_w^\alpha = p^\alpha = (n-1)^\alpha$, where w is the unique neighbor of u (which implies $d_w = n-1$). In other words, u is a pendent vertex of a star tree with n vertices. ■

In particular, for the first Zagreb index and the forgotten index, the problem of vertices with extremal local values is completely solved.

Corollary 1. *Let G be a graph with n non-isolated vertices and $u \in V\,(G)$. Then*

$$(2-n)\,(n-1)^2 + (n-1) \leq (\mathcal{R}_2)_G\,(u) \leq (n-1)^2\,. \tag{14}$$

Equality on the left side of (14) occurs if and only if u is the center of a star tree. Equality on the right of (14) occurs if and only if u is a pendent vertex of a star tree.

Corollary 2. *Let G be a graph with n non-isolated vertices and $u \in V\,(G)$. Then*

$$(2-n)\,(n-1)^3 + (n-1) \leq (\mathcal{R}_3)_G\,(u) \leq (n-1)^3\,. \tag{15}$$

Equality on the left side of (15) occurs if and only if u is the center of a star tree. Equality on the right of (15) occurs if and only if u is a pendent vertex of a star tree.

When $\alpha \in (0,1)$, the upper bound of $(\mathcal{R}_\alpha)_G\,(u)$ depends on the number of vertices of G, as we can see in our next example.

Example 6. Let G be a graph with n vertices.

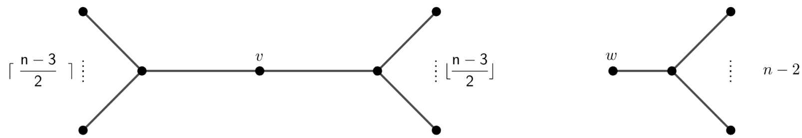

Figure 3. Vertices v, w used in Example 6.

1. If $n \leq 12$, then $h(x) = (1-x)\sqrt{x} + x\sqrt{\frac{n-1}{x}} \leq h(1) = \sqrt{n-1}$ for all $x \in [1, n-1] \cap \mathbb{N}$. Therefore, as in the proof of Theorem 6,

$$\left(\mathcal{R}_{\frac{1}{2}}\right)_G (u) \leq h(d_u) \leq h(1) = \sqrt{n-1}.$$

Hence if $n \leq 12$, then $\left(\mathcal{R}_{\frac{1}{2}}\right)_G (u)$ attains its maximal value when u is a pendent vertex of a star tree with n vertices. However, when $n \geq 13$, this is no longer true. In fact, consider the vertices v, w depicted in Figure 3. Then

$$\begin{aligned}\left(\mathcal{R}_{\frac{1}{2}}\right)_G (v) &= -\sqrt{2} + \sqrt{\lfloor \frac{n-3}{2} \rfloor + 1} + \sqrt{\lceil \frac{n-3}{2} \rceil + 1} \\ &> \sqrt{n-1} = \left(\mathcal{R}_{\frac{1}{2}}\right)_G (w),\end{aligned}$$

for all $n \geq 13$. In particular, a pendent vertex of a star tree is not maximal.

2. Similarly, when $\alpha < 0$, the minimal value of $(\mathcal{R}_\alpha)_G (u)$ depends on the number of vertices. For instance, consider the zeroth-order Randić index $\mathcal{R}_{-\frac{1}{2}}$. In this case, $h(x) = (1-x)\frac{1}{\sqrt{x}} + x\sqrt{\frac{x}{n-1}} \geq h(1)$ for all $x \in [1, n-1] \cap \mathbb{N}$ when $n \leq 7$. Hence,

$$\left(\mathcal{R}_{-\frac{1}{2}}\right)_G (u) \geq h(d_u) \geq h(1) = \sqrt{n-1},$$

so that $\left(\mathcal{R}_{-\frac{1}{2}}\right)_G (u)$ attains its minimal value when u is a pendent vertex of a star tree with n vertices. However, for the vertices v, w in Figure 3, $\left(\mathcal{R}_{-\frac{1}{2}}\right)_G (v) < \left(\mathcal{R}_{-\frac{1}{2}}\right)_G (w)$, for all $n \geq 8$, which implies that a pendent vertex of a star is not minimal.

So the following problem arises naturally:

1. Find vertices with maximal local value of the zeroth-order general Randić index $\mathcal{R}_\alpha$ when $0 < \alpha < 1$;

2. Find vertices with minimal local value of the zeroth-order general Randić index $\mathcal{R}_\alpha$ when $\alpha < 0$.

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