Graphs of Extremal Weights

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ABSTRACT. Our main aim is to show that the Randić weight of a connected graph of order n is at least $\sqrt{n-1}$. As shown by the stars, this bound is best possible.

Given adjacent vertices x and y of a graph, the *Randić weight* or simply *weight* of the edge xy is $R(xy) = (d(x)d(y))^{1/2}$, where $d(x)$ and $d(y)$ are the degrees of x and y. Also, the *Randić weight* or simply *weight* of a graph G, $R(G)$, is the sum of the weights of its edges. Randić [3] introduced this weight (which he called the *branching index*, and is now also called the *Randić index*) in his study of alkanes: he showed that there is a strong cörrelation between this index and chemical properties which critically depend on molecular size and shape (see [2]). Earlier, Wiener [4] had proposed for the same purpose an index he called the *path number*, which, for connected simple graphs, is the sum of all the distances between pairs of vertices.

The *Graffiti* program of Siemion Fajtlowicz has made numerous conjectures concerning, among others, the Randić weight of graphs with a given number of edges, and of graphs with a given number of non-isolated vertices.

James Shearer was the first to prove that the minimal Randić weight of a connected graph of order n goes to infinity with n. In fact, he proved in 1988 that the weight of a graph with n non-isolated vertices is at least

$\sqrt{n}/2$, and a little later Noga Alon improved this bound to $\sqrt{n}-8$ (see [1]). We shall show that the weight is, in fact, at least $\sqrt{n-1}$, the weight of a star with n vertices. The proof of this result is based on two easy lemmas.

Lemma 1. *Let x_1x_2 be an edge of a graph G of order n, with x_i having degree d_i. If $d_1 = 1$ then*

$$R(G) - R(G - x_1x_2) \geq \sqrt{d_2} - \sqrt{d_2 - 1} \geq \sqrt{n-1} - \sqrt{n-2}.$$

Proof: If $d_2 = 1$ then $R(G) - R(G - x_1x_2) = 1$; therefore we may and shall assume that $d_2 \geq 2$.

Denote by S_i the sum of the weights of the edges, other than x_1x_2, incident with the vertex x_i. Note that

$$R(G) - R(G - x_1x_2) = \frac{1}{\sqrt{d_2}} + S_2 - S_2\sqrt{\frac{d_2}{d_2 - 1}}.$$

Since $S_2 \leq (d_2 - 1)/\sqrt{d_2}$, we have

$$R(G) - R(G - x_1x_2) \geq \frac{1}{\sqrt{d_2}}\{1 + d_2 - 1 - \sqrt{d_2(d_2 - 1)}\} = \sqrt{d_2} - \sqrt{d_2 - 1}.$$

□

Lemma 2. *Let x_1x_2 be an edge of maximal weight in a graph G. Then*

$$R(G - x_1x_2) < R(G)$$

Proof: As in Lemma 1, for $i = 1, 2$ set $d_i = d(x_i)$ and denote by S_i the sum of the weights of the edges incident with x_i, except for the edge x_1x_2. If $\min\{d_1, d_2\} = 1$, then we are done by Lemma 1. Otherwise we have

$$S_i \leq (d_i - 1)/\sqrt{d_1d_2},$$

so

$$\begin{aligned}
&R(G) - R(G - x_1x_2) \\
&= \frac{1}{\sqrt{d_1d_2}} + S_1 + S_2 - S_1\sqrt{\frac{d_1}{d_1 - 1}} - S_2 - \sqrt{\frac{d_2}{d_2 - 1}} \\
&\geq \frac{1}{\sqrt{d_1d_2}}\left\{1 + (d_1 - 1)\left[1 - \sqrt{\frac{d_1}{d_1 - 1}}\right] + (d_2 - 1)\left[1 - \sqrt{\frac{d_2}{d_2 - 1}}\right]\right\} \\
&= \frac{1}{\sqrt{d_1d_2}}\left\{d_1 - \frac{1}{2} - \sqrt{d_1(d_1 - 1)} + d_2 - \frac{1}{2} - \sqrt{d_2(d_2 - 1)}\right\} > 0.
\end{aligned}$$

□

Our first main result easily follows from these two lemmas.

Theorem 3. *Let G be a graph of order n, containing no isolated vertex. Then*

$$R(G) \geq \sqrt{n-1}, \tag{1}$$

with equality if, and only if, G is a star.

Proof: If G is a star then we do have equality in (1), since each of the $n-1$ edges has weight $1/\sqrt{n-1}$.

To prove the main assertion of the theorem we apply induction on $n+m$, where m denotes the number of edges of G. It is trivial to check that the assertion holds for $n = 2, 3$, so let us assume that $n \geq 4$ and the result holds for smaller values of $n+m$.

Let x_1x_2 be an edge of maximal weight. By Lemma 1 and the induction hypothesis, we may assume that $G - x_1x_2$ has at least one isolated vertex.

If $G - x_1x_2$ has two isolated vertices (so that x_1x_2 is an isolated edge) then, by the induction hypothesis,

$$R(G) = 1 + R(G - x_1x_2) \geq 1 + \sqrt{n-3} > \sqrt{n-1}.$$

Suppose then that $G - x_1x_2$ has precisely one isolated vertex, say $d(x_1) = 1$ and $d(x_2) \geq 2$. Then, by Lemma 1 and the induction hypothesis,

$$R(G) \geq R(G - x_1x_2) + \sqrt{n-1} - \sqrt{n-2} \geq \sqrt{n-1}.$$

Furthermore, if the second of these inequalities is an equality then the graph $G - x_1x_2$ is a star of order $n-1$ and an isolated vertex. In that case G is either a star or else

$$R(G) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2(n-2)}} + \frac{n-3}{\sqrt{n-2}} > \sqrt{n-1}.$$

□

Before we turn to the minimal Randić weight of a graph with m edges, we consider another weighting. This time the weight of an edge is the product of the degrees of the endvertices, and we are interested in the maximal weight of a graph with m edges.

Theorem 4. *Let the weight of an edge $e = xy$ be $w(e) = d(x)d(y)$, and for a graph G set*

$$w(G) = \sum_{e \in E(G)} w(e).$$

Then every graph G of size $m = e(G)$ satisfies

$$w(G) \leq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^2. \tag{2}$$

Equality holds if, and only if, m is of the form $m = \binom{n}{2}$ for some natural number n and G is the union of K_n and isolated vertices.

Proof: Let G be a graph of size m, with vertex set $V(G) = \{x_1, \ldots, x_n\}$. For each i, $1 \le i \le n$, set $d_i = d(x_i)$ and $F(x_i) = V(G) - \Gamma(x_i) \cup \{x_i\}$. Thus $F(x_i)$ is the set of vertices *far* from x_i, at distance at least 2. Also, write e_i for the number of $\Gamma(x_i) - F(x_i)$ edges and f_i for the number of edges in $F(x_i)$. Note that

$$\sum_{x_j \in \Gamma(x_i)} d_j = 2m - d_i - e_i - 2f_i.$$

Consequently,

$$\begin{aligned} w(G) &= \frac{1}{2}\sum_{i=1}^{n} \sum_{x_j \in \Gamma(x_i)} w(x_i x_j) = \frac{1}{2}\sum_{i=1}^{n} d_i \sum_{x_j \in \Gamma(x_i)} d_j \\ &= \frac{1}{2}\sum_{i=1}^{n} d_i(2m - d_i - e_i - 2f_i) \\ &= 2m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i(d_i + e_i + 2f_i). \end{aligned} \tag{3}$$

Rather crudely,

$$d_i + e_i + f_i \ge \max\left\{d_i, m - \binom{d_i}{2}\right\} \ge \sqrt{8m+1} - 1,$$

so (3) gives that

$$\begin{aligned} w(G) &\le 2m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i\{\sqrt{8m+1} - 1\} \\ &= 2m^2 - m\{\sqrt{8m+1} - 1\} = m\left(\frac{\sqrt{8m+1} - 1}{2}\right)^2, \end{aligned}$$

as claimed.

For equality to hold in (2), we must have

$$d_i + e_i + f_i = d_i = m - \binom{d_i}{2},$$

whenever $d_i > 0$. Hence, G is a complete graph and isolated vertices. It is immediate that if G is a complete graph then we do have equality in (2), since if $m = \binom{n}{2}$ then $n - 1 = (\sqrt{8m+1} - 1)/2$. □

Theorem 4 easily implies analogous inequalities for more general weight. To be precise, for $\alpha \in \mathbb{R}$, $\alpha \neq 0$, define the weight $w_\alpha(e)$ of an edge e of a graph to be $w_\alpha(e) = (d(x)d(y))^\alpha$. Thus $w_1(e)$ is simply the weight $w(e)$ appearing in Theorem 4, and $w_{-1/2}(e)$ is the Randić weight of an edge. Also, set $w_\alpha(G) = \sum_{e \in E(G)} w_\alpha(e)$.

Theorem 5. *Every graph G of size m is such that*

$$w_\alpha(G) \leq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha} \tag{3}$$

for $0 < \alpha \leq 1$, and

$$w_\alpha(G) \geq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha} \tag{4}$$

for $-1 \leq \alpha < 0$. Furthermore, in (4) or (5) equality holds for a particular value of α if, and only if, G consists of a complete graph and isolated vertices, in which case we have equality in (4) and (5) for every α, $-1 \leq \alpha \leq 1$, $\alpha \neq 0$.

Proof: For $\alpha = 1$, the assertion is precisely Theorem 4, so we may assume that $\alpha \neq 1$. Suppose first that $0 < \alpha < 1$ and set $\beta = 1 - \alpha$, $p = 1/\alpha$, $q = 1/\beta$, so that $1/p + l/q = 1$. By Hölder's inequality and Theorem 4,

$$\begin{aligned} w_\alpha(G) &= \sum_e w(e)^\alpha \cdot 1^\beta \leq \left(\sum_e w(e)^{\alpha p}\right)^{1/p} \left(\sum_e 1\right)^{1/q} \\ &= w(G)^\alpha m^\beta \leq m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha}, \end{aligned}$$

implying(4). The case of equality follows from that in Theorem 4.

Inequality (5) is an immediate consequence of (4). Indeed, for $\alpha \neq 0$ we have

$$w_\alpha(G) w_{-\alpha}(G) \geq m^2,$$

since by the Cauchy-Schwartz inequality,

$$\begin{aligned} m &= \sum_e w_\alpha(e)^{1/2} w_{-\alpha}(e)^{1/2} \leq \left(\sum_e w_\alpha(e)\right)^{1/2} \left(\sum_e w_{-\alpha}(e)\right)^{1/2} \\ &= w_\alpha(G)^{1/2} w_{-\alpha}(G)^{1/2}. \end{aligned}$$

Therefore, by (4), if $1 \leq \alpha < 0$ then

$$m_\alpha(G) \geq m^2/m_{-\alpha}(G) \geq m^2/m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{-2\alpha} = m\left(\frac{\sqrt{8m+1}-1}{2}\right)^{2\alpha},$$

as claimed. The case of equality is again immediate. □

Perhaps the most interesting case of Theorem 5 is $\alpha = 1$. It is not unreasonable to expect that in this case one can determine the exact maximum of the weight of a graph with m edges. It is likely that if $\binom{n}{2} < m \leq \binom{n+1}{2}$ then the maximum is attained on a graph of order $n+1$ which contains a complete graph of order n.

As noted earlier, in the case $\alpha = -1/2$ we obtain precisely the Randić weight of a graph. Therefore if G is a graph with m edges then

$$R(G) \geq 2m/\{\sqrt{8m+1}-1\} = (\sqrt{8m+1}+1)/4. \qquad (5)$$

Also, equality holds in (6) if, and only if, G consists of a complete graph and isolated vertices.

Since the weight of an edge is at most 1, the weight of a graph with m edges is at most m. Our next aim is to determine the maximal weight of an r-uniform multigraph with n vertices, with the natural definition of the Randić weight.

To be precise, for $r \geq 1$, an *r-multiset on a set V* is a map $\rho\colon V \to \{0,1,\ldots,r\}$, with $\sum_{x\in V}\rho(x) = r$. We write $V^{(r)}$ for the set of all r-multisets on V. An *r-uniform multigraph* is a pair (V,m), where V, the *set of vertices*, is a finite set, and m is a map from $V^{(r)}$ to $[0,\infty)$. We think of $m(p)$ as the multiplicity of the 'edge' ρ.

The *degree* of a vertex x of a multigraph $G = (V,m)$ is

$$d(x) = \sum_{\rho\in V^{(r)}} m(\rho)\rho(x),$$

and the size of G is

$$e(G) = \sum_{\rho\in V^{(r)}} m(\rho) = \frac{1}{r}\sum_{x\in V} d(x).$$

Note that if $r = 2$, $m(\rho) = 0$ or 1, and $m(\rho) = 1$ implies that $\rho(x) = 0$ or 1 (and so $\rho(x) = \rho(y) = 1$ for two distinct vertices, and $\rho(z) = 0$ for every other vertex), then G is naturally identified with the graph (V,E), where $E = \{xy \in V^{(2)}\colon \rho(x) = \rho(y) = 1 \text{ for some } \rho \in V^{(2)} \text{ with } m(\rho) = 1\}$.

Define the *weight* of $\rho \in V^{(r)}$ to be

$$R(\rho) = \begin{cases} m(\rho)/\left(\Pi_{\rho(x)>0} d(x)^{\rho(x)}\right)^{1/r} & \text{if } m(\rho) > 0, \\ 0 & \text{otherwise.} \end{cases}$$

The *weight* $R(G)$ of an r-multigraph $G = (V,m)$ is the sum of the weights of its edges:

$$R(G) = \sum_{\rho\in V^{(r)}} R(\rho).$$

Theorem 6. *For $r \geq 1$, the weight of an r-multigraph G with n vertices is at most n/r. Furthermore, $R(G) = n/r$ if, and only if, G is d-regular for some $d > 0$, i.e. $d(x) = d > 0$ for every vertex x.*

Proof: If $G = (V, m)$ is d-regular for some $d > 0$ then $R(\rho) = m(\rho)/d$ for every $\rho \in V^{(r)}$, so

$$R(G) = \sum_{\rho \in V^{(r)}} R(\rho) = \frac{1}{d} \sum_{\rho \in V^{(r)}} m(\rho) = \frac{1}{dr} \sum_{x \in V} d(x) = n/r.$$

Now suppose that $G = (V, m)$ is an r-multigraph with n vertices, having k vertices of minimal degree $d > 0$, where $1 \leq k < n$. To prove the theorem, it suffices to show that there is a multigraph $G' = (V, m')$ with $R(G) < R(G')$, having at least $k+1$ vertices of minimal degree.

Set $U = \{u \in V : d(u) = d\}$ and let $e = \min\{d(v) : v \in V - U\}$. Define $m_0 : V^{(r)} \to [0, \infty)$ by

$$m_0(\rho) = \begin{cases} (e-d)/r & \text{if } \rho(u) = r \text{ for some } u \in U, \\ 0 & \text{otherwise,} \end{cases}$$

and set $G' = (V, m + m_0)$. Then G' has at least $k+1$ vertices of minimal degree e so to complete the proof, it suffices to show that $R(G') > R(G)$.

For simplicity, for $1 \leq i \leq r$, set $A_i = \{\rho \in V^{(r)} : \sum_{u \in U} \rho(u) = i\}$ and

$$a_i = \sum_{\rho \in A_i} m(\rho).$$

(Note that if G is an r-graph then a_i is the number of edges having precisely i vertices in U.) Clearly

$$\sum_{i=1}^{r} i a_i = \sum_{u \in U} d(u) = kd. \tag{6}$$

Also, writing $R(\rho)$ for the *weight in* G,

$$\begin{aligned} R(G') - R(G) &= \frac{k(e-d)}{re} + \sum_{i=1}^{r} \sum_{\rho \in A_i} R(\rho)\{(d/e)^{i/r} - 1\} \\ &\geq \frac{k(e-d)}{re} + \sum_{i=1}^{r} \sum_{\rho \in A_i} m(\rho)(d^i e^{r-i})^{-1/r}\{(d/e)^{i/r} - 1\} \\ &= \frac{k(e-d)}{re} - \frac{1}{e}\sum_{i=1}^{r}\{(e/d)^{i/r} - 1\} \sum_{\rho \in A_i} m(\rho) \\ &> \frac{k(e-d)}{re} - \frac{1}{e}\sum_{i=1}^{r}\left(\frac{e}{d} - 1\right)\frac{i}{r}a_i \\ &= \frac{k(e-d)}{re} - \frac{e-d}{edr}\sum_{i=1}^{r} i a_i = 0, \end{aligned}$$

where the final equality followed from (7). □

What can one say about the minimal weight of an r-graph with n non-isolated vertices? It seems likely that Theorem 3 can be generalized to the assertion that if an r-graph G has n non-isolated vertices then $R(G) \geq (n-r+1)^{1/r}$, with equality if, and only if, G consists of $n-r+1$ edges, sharing precisely the same $r-1$ vertices. Similarly, we conjecture that inequality (6) has the following extension: if G is an r-graph with $m = \binom{x}{r}$ edges then $R(G) \geq x/r$.

It would also be of interest to give a common refinement of Theorems 3 and 4, namely to determine the minimal weight of a graph containing m edges and n vertices of degree at least 1.

Finally, it is likely that Theorem 5 has a great many interesting extensions. First of all, a similar result is likely to hold for a variety of other edge-weights. However, for the weights w_α, the inequality $\alpha \leq 1$ is the natural boundary if we wish complete graphs to be extremal: for $\alpha > 1$ and large m complete graphs are no longer extremal. On a slightly different note, instead of giving weights to the edges, we may give weights to the complete r-graphs in our graph and then we may wish to maximize the total weight of a graph with n vertices or with m edges or with n vertices and m edges. For example, let the weight of a complete r-graph $K \subset G$ with vertex set $V(K) = \{x_1, \ldots, x_r\}$ be

$$\tilde{w}_r(K) = \prod_{i=1}^{r} d(x_i),$$

and let

$$\tilde{w}_r(G) = \sum \tilde{w}(K)$$

where the summation is over all r-graphs in G. Show that if $e(G) = \binom{n}{2}$ then, for $r \geq 2$, $\tilde{w}_r r(G) \leq \binom{n}{2}(n-1)^r$. We hope to return to these question in the near future.

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