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Double sun with largest Randić energy

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In 1975 Milan Randić introduced the Randić index, a molecular structure descriptor, defined as $R_{-\frac{1}{2}}(G) = \sum_{i\sim j} \frac{1}{\sqrt{d_i d_j}}$, where the summation is over all pairs of adjacent vertices of the graph. This index has applications in chemistry and pharmacology and has been extensively studied in mathematics and mathematical chemistry. Furthermore, the Randić index motivated the association to a graph G the symmetric matrix of order n, called Randić matrix, and its energy, which meets important applications in real world problems in chemistry.

Let $G = (V, E)$ be a simple undirected graph of order n. The Randić matrix $R(G) = [r_{ij}]$ of G is defined as $\frac{1}{\sqrt{d_i d_j}}$ if $ij \in E$ and 0 otherwise. The Randić energy of G is defined as $RE(G) = \sum_{i=1}^{n} |\lambda_i|$ where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $R(G)$. Notice that, the normalized Laplacian matrix of a graph G can be written using the Randić matrix as $\mathcal{L}(G) = I_n - R(G)$. And, for graphs without isolated vertices, the normalized Laplacian energy is given by $E_{\mathcal{L}}(G) = \sum_{i=1}^{n} |\mu_i - 1|$ where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of $\mathcal{L}$. By way of mativation, we would like to point out that if G is a graph without isolated vertices then $RE(G) = E_{\mathcal{L}}(G)$. Finding the graph having the largest (or the smallest) Randić energy is not only an important applied problem, but it is a beautiful mathematical problem per se.

In [2], Gutman, Furtula and Bozkurt used computational experiments to conjecture that the sun and the double sun are the graphs with largest Randić energy among connected graphs. The p-sun, S^p, is a starlike tree of order $n = 2p + 1$, $p \geq 0$, havin p-paths of length 2, as illustrated on the left side of Figure 1. The (p, q)-double sun, $D^{p,q}$, is a tree of order $n = 2(p + q + 1)$, where $p, q \geq 0$, obtained by connecting the centers of a p-sun and a q-sun with an edge, as depicted on the right side of Figure 1. The (p, q)-double sun is said balanced if $|p - q| \leq 1$. Since then, very little progress is being made on proving the conjecture.

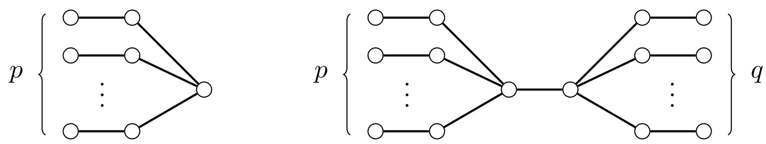

Figure 1: p-sun and (p, q)-double sun.

In this note, we show that the $(\lceil \frac{n-2}{4} \rceil, \lfloor \frac{n-2}{4} \rfloor)$-double sun attains the largest Randić energy among the (p, q)-double suns of order $n = 2(p + q + 1)$, partially proving the conjecture. More precisely we prove the following result.

Theorem 1. *For an even number $n = 2(p + q + 1) \geq 8$ with $p,q \geq 0$, the (p, q)-double sun attains the maximum energy when $p = \lceil \frac{n-2}{4} \rceil$ and $q = \lfloor \frac{n-2}{4} \rfloor$.*

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The characteristic polynomial of the (p, q)-double sun, presented in [1], is given by

$$P(\lambda) = \lambda(\lambda - 2)\left(\lambda - \left(\frac{2+\sqrt{2}}{2}\right)\right)^{p+q-2}\left(\lambda - \left(\frac{2-\sqrt{2}}{2}\right)\right)^{p+q-2}(\alpha(\lambda)) \tag{1}$$

where $\alpha(\lambda) = \lambda^4 - 4\lambda^3 + \frac{(20pq+22p+22q+20)}{4(p+1)(q+1)}\lambda^2 + \frac{(-8pq-12p-12q-8)}{4(p+1)(q+1)}\lambda + \frac{2p+2q+1}{4(p+1)(q+1)}$.

After some algebraic manipulation the Randić energy of the $D^{p,q}$ can be written as

$$RE(D^{p,q}) = 2 + \sqrt{2}\,(p+q-2) + \frac{\sqrt{(p+1)(q+1)}}{(p+1)(q+1)}\sqrt{4\,pq + 2\,p + 2\,q + 4 + 4\,\sqrt{pq+p+q+1}}. \tag{2}$$

Next, we replace $q = \frac{n-2p-2}{2}$ in (2) and we obtain

$$2 + \sqrt{2}\left(\frac{n}{2} - 3\right) + \frac{\sqrt{(p+1)\left(\frac{n}{2} - p\right)}\sqrt{4\,p\left(\frac{n}{2} - p - 1\right) + n + 2 + 4\,\sqrt{p\left(\frac{n}{2} - p - 1\right) + \frac{n}{2}}}}{(p+1)\left(\frac{n}{2} - p\right)}. \tag{3}$$

Note that $RE(D^{p,q}) = RE(p)$ can be manipulated as a function of p with domain $0 \le p \le \frac{n-2}{2}$. Therefore, using the first derivative test, we can find the maximum point of $RE(p)$. The derivative of $RE(p)$ with respect to p, $RE^{'}(p)$, is given by

$$-\frac{1}{2}\,\frac{\sqrt{2}\,(n-4\,p-2)\left(\sqrt{2}\sqrt{(p+1)\,(n-2\,p)} - n + 2\right)}{\sqrt{2\,\sqrt{2}\sqrt{(p+1)\,(n-2\,p)} + 2\,pn - 4\,p^2 + n - 4\,p + 2}\sqrt{(p+1)\,(n-2\,p)}\,(p+1)\,(n-2\,p)}. \tag{4}$$

Now, we analyse the numerator and denominator of $RE^{'}(p)$. First, it is straightforward to return to the variables p and q in the denominator of $RE^{'}(p)$ to show that it is always positive. Next, we analyse the numerator. We have the factor $-\sqrt{2}$ and $\sqrt{2}\sqrt{(p+1)\,(n-2\,p)} - n + 2$ that is negative when $n > 6$. Therefore, the sign of $RE^{'}(p)$ is given by the linear function $n - 4p - 2$. Then $RE^{'}(p) > 0$ if $p < \frac{n-2}{4}$, $RE^{'}(p) = 0$ if $p = \frac{n-2}{4}$ and $RE^{'}(p) < 0$ if $p > \frac{n-2}{4}$. Hence, given n even and $n \ge 8$, we have that $p = \frac{n-2}{4}$ is maximum point of $RE(p)$.

Observe that when $p = \frac{n-2}{4}$ we have that $q = \frac{n-2}{4}$. Note that, p is an integer number when $n = 4k + 2$, for any integer $k \ge 2$. Then, we still have to analyze when $n = 4k$ and consequently p is not an integer number. If $n = 4k$, we have that $k - 1 = \lfloor k - \frac{1}{2} \rfloor \le p = k - \frac{1}{2} \le \lceil k - \frac{1}{2} \rceil = k$. Now, if $p = k - 1$ then $q = k$, and if $p = k$ then $q = k - 1$. Replacing these values in (2) we obtain that $RE(D^{k-1,k}) = RE(D^{k,k-1})$. Therefore, when $n = 4k$ the integer that returns the largest $RE(p)$ is $p = k$ or $p = k - 1$. Now, we can assume that $p \ge q$ and if $n = 4k$, the maximum of $RE(p)$ is attained when we take the ceiling of $p = \frac{n-2}{4}$ and the floor of $q = \frac{n-2}{4}$.

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