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Unicycle graphs with maximum generalized topological indices*

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Let G be an unicycle graph and d_v the degree of the vertex v. In this paper, we investigate the following topological indices for an unicycle graph G: $\alpha_m(G) = \sum_{v\in V(G)} {d_v}^m$, $\alpha_{-m}(G) = \sum_{v\in V(G)} {d_v}^{-m}$, $\alpha_{-\frac{1}{m}}(G) = \sum_{v\in V(G)} {d_v}^{-\frac{1}{m}}$, where $m \geqslant 2$ is an integer. All unicycle graphs with the largest values of the three topological indices are characterized.

KEY WORDS: Unicyclic graph, the generalied topological index, the Zeroth-order Randic index

1. Introduction

Let $G = (V(G), E(G))$ denote a graph with $V(G)$ as the set of vertices and $E(G)$ as the set of edges. $N_G(v_i)$ denotes the neighbors of v_i. The Randić index of G defined in [1] is

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

where $d_v = d_G(v)$ denotes the degree of the vertex v in G. Randić demonstrated that his index is well correlated with a variety of Physic-Chemical properties of an alkane. The index χ became one of the most popular molecular descriptors. See [1–6], the zeroth-order Randić index $\chi^0(G)$ of G defined by Kier and Hall [7] is $\chi^0(G) = \sum_{v\in V(G)} \frac{1}{\sqrt{d_v}}$. Pavlović [6] gave the unique graph with largest value of $\chi^0(G)$. In [8], Lielal investigated the same problem for the topological index $M_1(G)$, a Zagreb index [9], which is defined as $M_1(G) = \sum_{v\in V(G)} {d_v}^2$. By observing the common appearance of the Randić index and the Zagreb index, In [10], Xueliang Li and Haixing Zhao has described the following four general topological indices:

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(i) $\alpha_m(G) = \sum_{v\in V(G)} d_v{}^m$,

(ii) $\alpha_{-m}(G) = \sum_{v\in V(G)} d_v{}^{-m}$,

(iii) $\alpha_{-\frac{1}{m}}(G) = \sum_{v\in V(G)} d_v{}^{-\frac{1}{m}}$,

(iv) $\alpha_{\frac{1}{m}}(G) = \sum_{v\in V(G)} d_v{}^{\frac{1}{m}}$,

where m is a positive integer usually at least 2. In [10], all trees with the smallest, the second and third smallest values of the four topological indices are characterized. The same is done for all trees with largest, the second and third largest values of these indices. In this paper, we will investigate the forth three general topological indices for the unicycle graphs and all unicycle graphs with the largest values of these topological indices are characterized.

Throughout this paper, we consider finite and simple graphs only. We denote, respectively, by S_n, P_n and C_n the star, path and cycle with n vertices. By $S_{n-k+3} + P_{k-1}$ we denote the unicycle graph of order n which has a cycle of length k and the other vertices are adjacent to the same vertex on the cycle, as shown in figure 1. Let $\mathcal{U}_n$ denote the set of all unicycle graphs of order n. By $\mathcal{U}_n^k$ we denote the set of the unicycle graphs in which the length of its cycle is k. Undefined notations and terminology will conform to those in [10].

2. The unicycle graphs with maximum values of the three indices

For convenience, we introduce two transfer operations.

Transfer operation A: Let G be an unicycle graph in $\mathcal{U}_n^k$, $C_k = v_1v_2v_3\cdots v_kv_1$ is the unique cycle of G. If there are i and j such that $1 \leqslant i < j \leqslant k$ and $d_G(v_i) = p+2$, $d_G(v_j) = q+2$,$p, q \geqslant 1$, $N_G(v_i) = \{v_{i-1}, v_{i+1}, u_1, u_2, \ldots, u_p\}$, $N_G(v_j) = \{v_{j-1}, v_{j+1}, w_1, w_2, \ldots, w_q\}$, then G is changed into G' after the transfer operation A, where $G' = G - \{v_iu_1, v_iu_2, \ldots, v_iu_p\} + \{v_ju_1, v_ju_2, \ldots, v_ju_p\}$. As shown in figure 2.

Remark. Repeating the above operations, any graph G in $\mathcal{U}_n^k$ must be changed into a graph which has at most one vertex with degree greater than 2.

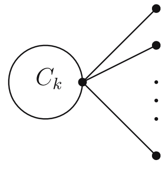

Figure 1.

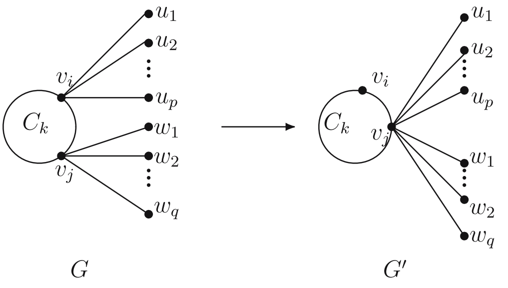

Figure 2.

Lemma 1. If G is changed into G' after the transfer operation A, then

(i) $\alpha_m(G') > \alpha_m(G)$;

(ii) $\alpha_{-m}(G') > \alpha_{-m}(G)$;

(iii) $\alpha_{-\frac{1}{m}}(G') > \alpha_{-\frac{1}{m}}(G)$.

Proof. Note that

$$
\begin{aligned}
\text{(i) } \alpha_m(G') - \alpha_m(G) &= [(p+q+2)^m + 2^m] - [(p+2)^m + (q+2)^m] \\
&= [(p+q+2)^m - (p+2)^m] - [(q+2)^m - 2^m] \\
&= mq\xi^{m-1} - mq\eta^{m-1} (\xi \in [p+2, p+2+q], \quad \eta \in [2, q+2]) \\
&= mq(\xi^{m-1} - \eta^{m-1}) \\
&> 0,
\end{aligned}
$$

$$
\begin{aligned}
\text{(ii) } \alpha_{-m}(G') - \alpha_{-m}(G) &= [(p+q+2)^{-m} + 2^{-m}] - [(p+2)^{-m} + (q+2)^{-m}] \\
&= [(p+q+2)^{-m} - (p+2)^{-m}] - [(q+2)^{-m} - 2^{-m}] \\
&= -mq\xi^{-m-1} + mq\eta^{-m-1} \quad (\xi \in [p+2, p+2+q], \\
&\qquad \eta \in [2, q+2]) \\
&= -mq(\xi^{-m-1} - \eta^{-m-1}) \\
&> 0
\end{aligned}
$$

$$
\begin{aligned}
\text{(iii) } \alpha_{-\frac{1}{m}}(G') - \alpha_{-\frac{1}{m}}(G) &= [(p+q+2)^{-\frac{1}{m}} + 2^{-\frac{1}{m}}] - [(p+2)^{-\frac{1}{m}} + (q+2)^{-\frac{1}{m}}] \\
&= [(p+q+2)^{-\frac{1}{m}} - (p+2)^{-\frac{1}{m}}] - [(q+2)^{-\frac{1}{m}} - 2^{-\frac{1}{m}}] \\
&= -\frac{1}{m}q\xi^{-\frac{1}{m}} + \frac{1}{m}q\eta^{-\frac{1}{m}} \quad (\xi \in [p+2, p+2+q], \\
&\quad \eta \in [2, q+2]) \\
&= -\frac{1}{m}q(\xi^{-\frac{1}{m}} - \eta^{-\frac{1}{m}}) \\
&> 0
\end{aligned}
$$

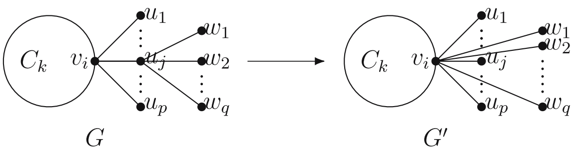

Figure 3.

So, the proof of Lemma 1 is completed.

Transfer operation B. Let $G \in \mathcal{U}_n^k$, $C_k = v_1v_2v_3\cdots v_kv_1$ is the unique cycle of G. There is only one vertex v_i with degree more than 2 on the cycle C_k, and $d_G(v_i) = p+2 > 2$, $N_G(v_i) = \{v_{i-1}, v_{i+1}, u_1, u_2, \ldots, u_p\}$. If there is j $(1 \leqslant j \leqslant p)$ such that $d_G(u_j) = q+1 \geqslant 2$, and $N_G(u_j) = \{v_i, w_1, w_2, \ldots, w_q\}$, then G is changed into G' after the transfer operation B, where $G' = G - \{u_jw_1, u_jw_2, \ldots, u_jw_q\} + \{v_iw_1, v_iw_2, \ldots, v_iw_q\}$. As shown in figure 3.

Lemma 2. If G is changed into G' after the transfer operation B, then

(i) $\alpha_m(G') > \alpha_m(G)$;

(ii) $\alpha_{-m}(G') > \alpha_{-m}(G)$;

(iii) $\alpha_{-\frac{1}{m}}(G') > \alpha_{-\frac{1}{m}}(G)$.

Proof. Note that

$$
\begin{aligned}
\text{(i) } \alpha_m(G') - \alpha_m(G) &= [(p+2+q)^m + 1] - [(p+2)^m + (q+1)^m] \\
&= [(p+2+q)^m - (p+2)^m] - [(q+1)^m - 1] \\
&= mq\xi^{m-1} - mq\eta^{m-1} \;\; (\xi \in [p+2, p+2+q],\;\; \eta \in [1, q+1]) \\
&= mq(\xi^{m-1} - \eta^{m-1}) \\
&> 0,
\end{aligned}
$$

$$
\begin{aligned}
\text{(ii) } \alpha_{-m}(G') - \alpha_{-m}(G) &= [(p+2+q)^{-m} + 1] - [(p+2)^{-m} + (q+1)^{-m}] \\
&= [(p+2+q)^{-m} - (p+2)^{-m}] - [(q+1)^{-m} - 1] \\
&= -mq\xi^{-m-1} + qm\eta^{-m-1} \;\; (\xi \in [p+2, p+2+q], \\
&\quad\; \eta \in [1, q+1]) \\
&= -mq(\xi^{-m-1} - \eta^{-m-1}) \\
&> 0,
\end{aligned}
$$

$$
\begin{aligned}
\text{(iii) } \alpha_{-\frac{1}{m}}(G') - \alpha_{-\frac{1}{m}}(G) &= [(p+2+q)^{-\frac{1}{m}} + 1] - [(p+2)^{-\frac{1}{m}} + (q+1)^{-\frac{1}{m}}] \\
&= [(p+2+q)^{-\frac{1}{m}} - (p+2)^{-\frac{1}{m}}] - [(q+1)^{-\frac{1}{m}} - 1] \\
&= -\frac{1}{m}q\xi^{-\frac{1}{m}-1} - \frac{1}{m}q\eta^{-\frac{1}{m}-1}
\end{aligned}
$$

$$
\begin{aligned}
&\times (\xi \in [p+2, p+2+q], \eta \in [1, q+1]) \\
&= -\frac{1}{m} q (\xi^{-\frac{1}{m}-1} - \eta^{-\frac{1}{m}-1}) \\
&> 0.
\end{aligned}
$$

So, the proof of Lemma 2 is completed.

In the following, we shall investigate the unicycle graphs with maximum values of the three indices.

Theorem 1. $S_{n-k+3} + P_{k-1}$ is the unique unicycle graph in $\mathcal{U}_n^k$ with maximum values of the three topological indices.

Proof. For any G in $\mathcal{U}_n^k$, we can obtain a graph G' in $\mathcal{U}_n^k$ from G by a series of transfer operations A, such that G' has at most one vertex with degree greater than 2 on its cycle. Then, $S_{n-k+3} + P_{k-1}$ can be also obtained from G' by a series of transfer operations B. So the unicycle graph in $\mathcal{U}_n^k$ with maximum values of the three topological indices is $S_{n-k+3} + P_{k-1}$ by Lemmas 1 and 2, and the theorem is thus proved.

Theorem 2. $S_n + P_1$ is the unique unicycle graph in $\mathcal{U}_n$ with maximum values of the three topological indices.

Proof. If $3 \leqslant k < k' \leqslant n$, then

$$
\begin{aligned}
&\alpha_m(S_{n-k'+3} + P_{k'-1}) - \alpha_m(S_{n-k+3} + P_{k-1}) \\
&\quad = [2^m(k'-1) + (2+n-k')^m + n - k'] - [2^m(k-1) + (2+n-k)^m + n - k] \\
&\quad = (k'-k)[2^m - 1 + (2+n-k')^m - (2+n-k)^m] \\
&\quad = (k'-k)(m\eta^{m-1} - m\xi^{m-1})(\eta \in [1,2], \quad \xi \in [2+n-k', 2+n-k]) \\
&\quad = m(k'-k)(\eta^{m-1} - \xi^{m-1}) \\
&\quad < 0
\end{aligned}
$$

So, $\alpha_m(S_{n-k'+3} + P_{k'-1}) < \alpha_m(S_{n-k+3} + P_{k-1})$.

Similarly, we have

$\alpha_{-m}(S_{n-k'+3}+P_{k'-1})<\alpha_{-m}(S_{n-k+3}+P_{k-1})$, $\alpha_{-\frac{1}{m}}(S_{n-k'+3}+P_{k'-1}) < \alpha_{-\frac{1}{m}}(S_{n-k+3}+P_{k-1})$.

From Theorem 1, we can see that the unicycle graph with maximum values of three general topological indices must be $S_{n-k+3} + P_{k-1}$, and the theorem is thus proved. □

References

[1] M. Randić, J. Math. Chem. 24 (1998) 345–358.
[2] O. Araujo and J. Rada, J. Math. Chem. 27 (2000) 19–30.

[3] E. Esrrada, Chem. Phys. Lett. 336 (2001) 248–252.
[4] M. Fishermann, I. Gutman, A. Hoffmann, D. Rautenbach, D. Vidoić and L. Volkmann, Z. Naturforsch 57a (2002) 49–52.
[5] M. Randić, J. Am. Chem. Soc. 97 (1975) 6609–6615.
[6] L. Pavlovič, Discrete Appl. Math. 127 (2003) 615–626.
[7] L.B. Kier and L. Hall, *Molecular Connectivity in Structure Activity Analysis* (Research Studies Press, Wiley, Chichester, UK, 1986).
[8] P. Hansen and H. Mélot, J. Chem. Inf. Comput. Sci. 43 (2003) 1–14.
[9] N. Trinajstic, *Chemical Graph Theory* (CRC press, 1992).
[10] X.L. Li and H.X. Zhao, MATCH Commun. Math. Comput. Chem. 51 (2004) 205–210.
[11] I. Gutman and O. Miljković, Chem. Phys. Lett. 306 (1999) 366–372.