ON A CONJECTURE OF MERRIFIELD AND SIMMONS

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Abstract

Let $\sigma(G)$ be the number of independent-vertex sets of a graph G. Merrifield and Simmons conjectured that for any graph G and any pair of non-adjacent vertices u and v of G,

$$\sigma(G-u)\sigma(G-v)-\sigma(G)\sigma(G-u-v)\begin{cases} >0 & \text{if } d(u,v) \text{ is odd} \\ <0 & \text{if } d(u,v) \text{ is even}\end{cases}$$

where $d(u,v)$ denotes the distance of u and v in G. Gutman proved that the conjecture is true for all trees. In the present paper, we prove that the conjecture is true for all cycles and many other kinds of graphs. Unfortunately, we find families of examples showing that the conjecture is not true in general.

1. Introduction.

Let G be a (molecular) graph. The vertex set and edge set of G are denoted by $V(G)$ and $E(G)$, respectively. Two vertices of G are said to be independent if they are not adjacent. The k-th independence number of G is denoted by $\sigma_k(G)$. By definition, for $k \geq 2$, $\sigma_k(G)$ is equal to the number of ways in which k pairwise independent vertices can be selected in the graph G. In addition to this, $\sigma_0(G) = 1$ and $\sigma_1(G) = |V(G)|$. The k-th clique number $c_k(G)$ of G is defined to be the number of ways in which k pairwise adjacent vertices can be selected in the graph G ($k \geq 2$). In addition to this, $c_0(G) = 1$, $c_1(G) = |V(G)|$; note that $c_2(G) = |E(G)|$.

Let $\sigma(G) = \sum_{k\geq 0}\sigma_k(G)$, the number of independent-vertex sets of G, and $c(G) = \sum_{k\geq 0} c_k(G)$, the number of cliques of G. It is easily seen that $c(\overline{G}) = \sigma(G)$, where $\overline{G}$ denotes the complement of G. The quantity $\sigma(G)$ was extensively studied in connection with certain topological problems of chemistry [3]. On page 144 of [3], Merrifield and Simmons stated without proof a property of $\sigma(G)$ (see Gutman[1]), which for nonadjacent vertices u and v can be formulated as follows:

$$\Delta_{uv}(G) = \sigma(G-u)\sigma(G-v) - \sigma(G)\sigma(G-u-v)$$

* Partially supported by NSFC.

$$\begin{cases} > 0, & if\ d(u,v)\ is\ odd \\ < 0, & if\ d(u,v)\ is\ even, \end{cases} \qquad \textbf{(Assertion)}$$

where $d(u,v)$ (or $d_G(u,v)$) denotes the distance of u and v in G. Gutman proved [1] that this **Assertion** is true at least for all trees. In this paper, we prove that this **Assertion** is true for cycles and many other kinds of graphs. However, we find infinitely many examples showing that the **Assertion** is not true in general.

Since $c(\overline{G}) = \sigma(G)$, we have

$$\Delta_{uv}(G) = c(\overline{G-u})c(\overline{G-v}) - c(\overline{G})c(\overline{G-u-v}).$$

Sometimes, the right-hand side of the above equality is easier to calculate.

2. Proof for Cycles and Other Kinds of Graphs..

Let C_n denote the cycle with n vertices and P_n the path with n vertices. From [2] we know that

$$\sigma(P_n) = \sigma(P_{n-1}) + \sigma(P_{n-2}) \qquad (*)$$

with $\sigma(P_0) = 1$ and $\sigma(P_1) = 2$, which is exactly the Fibonacci sequence. In order to prove that **Assertion** for cycles, we need the following properties of $\sigma(P_n)$.

Property 1: Let k be a positive integer with $1 \leq k \leq n-2$. Then from page 203 of [3] we have $\sigma(P_n) = \sigma(P_k)\sigma(P_{n-k-1}) + \sigma(P_{k-1})\sigma(P_{n-k-2})$. Note that here $\sigma(P_n) = F_{n+1}$.

Property 2: From property (*), we can obtain that

$$\begin{aligned} &\sigma(P_{2k-1})\sigma(P_{n-2k-3}) - \sigma(P_{2k})\sigma(P_{n-2k-4}) \\ &= \sigma(P_{2k-3})\sigma(P_{n-2k-5}) - \sigma(P_{2k-2})\sigma(P_{n-2k-6}). \end{aligned}$$

Hence, if $n \geq 4k+2$, from the above recursive relation we can get that

$$\begin{aligned} &\sigma(P_{2k-1})\sigma(P_{n-2k-3}) - \sigma(P_{2k})\sigma(P_{n-2k-4}) \\ &= \sigma(P_1)\sigma(P_{n-4k-1}) - \sigma(P_2)\sigma(P_{n-4k-2}) \\ &= 2\sigma(P_{n-4k-1}) - 3\sigma(P_{n-4k-2}) \\ &= \begin{cases} 2\sigma(P_1) - 3\sigma(P_0) = 1 > 0, & if\ n = 4k+2 \\ 2\sigma(P_{n-4k-3}) - \sigma(P_{n-4k-2}) > 0, & if\ n > 4k+2 \end{cases} \\ &\quad (\text{since } \sigma(P_m) < 2\sigma(P_{m-1}) \text{ for any } m \geq 1) \end{aligned}$$

Property 3: Also, from property (*), we can get that

$$\sigma^2(P_{2k-1}) - \sigma(P_{2k})\sigma(P_{2k-2}) = \sigma^2(P_{2k-3}) - \sigma(P_{2k-2})\sigma(P_{2k-4}).$$

Hence,

$$\sigma^2(P_{2k-1}) - \sigma(P_{2k})\sigma(P_{2k-2}) = \sigma^2(P_1) - \sigma(P_2)\sigma(P_0) = 4 - 3 = 1 > 0.$$

Similarly, we have

$$\begin{aligned}
&\sigma^2(P_{2k}) - \sigma(P_{2k+1})\sigma(P_{2k-1}) \\
&= \sigma^2(P_{2k-2}) - \sigma(P_{2k-1})\sigma(P_{2k-3}) \\
&= \sigma^2(P_2) - \sigma(P_3)\sigma(P_1) \\
&= 9 - 10 = -1 < 0.
\end{aligned}$$

Theorem: Let $u, v \in V(C_n)$ and $uv \notin E(C_n)$. Then we have

$$\Delta_{uv}(C_n)\begin{cases} > 0 & \text{if } d_{C_n}(u,v) \text{ is odd} \\ < 0 & \text{if } d_{C_n}(u,v) \text{ is even.} \end{cases}$$

Proof: From [2], we have

$$\sigma(C_n) = \sigma(P_{n-1}) + \sigma(P_{n-3}).$$

Thus,

$$\Delta_{uv}(C_n) = \sigma^2(P_{n-1}) - [\sigma(P_{n-1}) + \sigma(P_{n-3})]\sigma(P_r)\sigma(P_l),$$

where $r + l = n - 2$ with $r > 0$ and $l > 0$.

It is clear that $d(u,v) = min\{r,l\} + 1$. Without loss of generality, we assume that $r \leq l$ and therefore $d(u,v) = r + 1$.

If $r = 1$,

$$\begin{aligned}
&\Delta_{uv}(C_n) \\
=&\sigma^2(P_{n-1}) - [\sigma(P_{n-1}) + \sigma(P_{n-3})]\sigma(P_1)\sigma(P_{n-3}) \\
=&\sigma^2(P_{n-1}) - 2\sigma(P_{n-1})\sigma(P_{n-3}) - 2\sigma^2(P_{n-3}) \\
=&[\sigma(P_{n-1}) - \sigma(P_{n-3})]^2 - 3\sigma^2(P_{n-3}) \\
=&\sigma^2(P_{n-2}) - 3\sigma^2(P_{n-3}) \\
=&-2\sigma^2(P_{n-3}) + 2\sigma(P_{n-3})\sigma(P_{n-4}) + \sigma^2(P_{n-4}) \\
=&2\sigma(P_{n-3})[\sigma(P_{n-4}) - \sigma(P_{n-3})] + \sigma^2(P_{n-4}) \\
=&-2\sigma(P_{n-3})\sigma(P_{n-5}) + \sigma^2(P_{n-4}) \\
<&-\sigma(P_{n-3})\sigma(P_{n-4}) + \sigma^2(P_{n-4}) \\
&(\text{ since } \sigma(P_{n-4}) < 2\sigma(P_{n-5})) \\
<&0 \\
&(\text{ since } \sigma(P_{n-4}) < \sigma(P_{n-3})).
\end{aligned}$$

Hence, the theorem is true for $r = 1$.

Now, we distinguish the following two cases.

Case 1: $r = 2k$ $(k \geq 1)$, $(n = r + l + 2 \geq 4k + 2)$.

Then

$$
\begin{aligned}
&\Delta_{uv}(C_n) \\
=&\sigma^2(P_{n-1}) - [\sigma(P_{n-1}) + \sigma(P_{n-3})]\sigma(P_{2k})\sigma(P_{n-2k-2}) \\
=&\sigma^2(P_{n-1}) - \sigma(P_{n-1})\sigma(P_{2k})\sigma(P_{n-2k-2}) - \sigma(P_{n-3})\sigma(P_{2k})\sigma(P_{n-2k-2}) \\
=&\sigma(P_{n-1})[\sigma(P_{n-1}) - \sigma(P_{2k})\sigma(P_{n-2k-2})] - \sigma(P_{n-3})\sigma(P_{n-2k-2})\sigma(P_{2k}) \\
=&[\sigma(P_{2k})\sigma(P_{n-2k-2}) + \sigma(P_{2k-1})\sigma(P_{n-2k-3})]\sigma(P_{2k-1})\sigma(P_{n-2k-3}) \\
&- [\sigma(P_{n-2k-2})\sigma(P_{2k-2}) + \sigma(P_{n-2k-3})\sigma(P_{2k-3})]\sigma(P_{n-2k-2})\sigma(P_{2k}) \\
&(\textit{ using Property 1 for } \sigma(P_{n-1}) \textit{ and } \sigma(P_{n-3})\ ) \\
=&\sigma^2(P_{2k-1})\sigma^2(P_{n-2k-3}) + \sigma(P_{2k})\sigma(P_{2k-1})\sigma(P_{n-2k-2})\sigma(P_{n-2k-3}) \\
&- \sigma(P_{2k-3})\sigma(P_{2k})\sigma(P_{n-2k-3})\sigma(P_{n-2k-2}) - \sigma(P_{2k-2})\sigma(P_{2k})\sigma^2(P_{n-2k-2}) \\
=&\sigma^2(P_{2k-1})\sigma^2(P_{n-2k-3}) + \sigma(P_{2k})\sigma(P_{2k-2})\sigma(P_{n-2k-2})\sigma(P_{n-2k-3}) \\
&- \sigma(P_{2k-2})\sigma(P_{2k})\sigma^2(P_{n-2k-2}) \\
&(\textit{ since } \sigma(P_{2k-1}) - \sigma(P_{2k-3}) = \sigma(P_{2k-2})) \\
=&\sigma^2(P_{2k-1})\sigma^2(P_{n-2k-3}) - \sigma(P_{2k})\sigma(P_{2k-2})\sigma(P_{n-2k-2})\sigma(P_{n-2k-4}) \\
&(\textit{ since } \sigma(P_{n-2k-3}) - \sigma(P_{n-2k-2}) = -\sigma(P_{n-2k-4})) \\
=&\sigma^2(P_{2k-1})\sigma^2(P_{n-2k-3}) - \sigma(P_{2k-2})\sigma(P_{2k})\sigma(P_{n-2k-4})\sigma(P_{n-2k-3}) \\
&- \sigma(P_{2k})\sigma(P_{2k-2})\sigma^2(P_{n-2k-4}) \\
&(\textit{ since } \sigma(P_{n-2k-2}) = \sigma(P_{n-2k-3}) + \sigma(P_{n-2k-4})) \\
=&[\sigma(P_{2k-1})\sigma(P_{n-2k-3}) + \sigma(P_{2k-2})\sigma(P_{n-2k-4})][\sigma(P_{2k-1})\sigma(P_{n-2k-3}) \\
&- \sigma(P_{2k})\sigma(P_{n-2k-4})] + [\sigma^2(P_{2k-1}) \\
&- \sigma(P_{2k})\sigma(P_{2k-2})]\sigma(P_{n-2k-4})\sigma(P_{n-2k-3}) \\
>&0, \\
&(\textit{ from Properties 2 and 3})
\end{aligned}
$$

i.e., $\Delta_{uv}(C_n) > 0$, for $d(u, v) = r + 1 = 2k + 1$ (*odd*). Thus, the theorem is true for $r = 2k$.

Case2: $r = 2k + 1$ $(k \geq 1)$ $(n = r + l + 2 \geq 4k + 4)$.

Then

$$
\begin{aligned}
&\Delta_{uv}(C_n) \\
=&\sigma^2(P_{n-1}) - [\sigma(P_{n-1}) + \sigma(P_{n-3})]\sigma(P_{2k+1})\sigma(P_{n-2k-3}) \\
=&\sigma(P_{n-1})[\sigma(P_{n-1}) - \sigma(P_{2k+1})\sigma(P_{n-2k-3})] - \sigma(P_{n-3})\sigma(P_{n-2k-3})\sigma(P_{2k+1}) \\
=&[\sigma(P_{2k})\sigma(P_{n-2k-4}) + \sigma(P_{2k+1})\sigma(P_{n-2k-3})]\sigma(P_{2k})\sigma(P_{n-2k-4}) \\
&- [\sigma(P_{n-2k-3})\sigma(P_{2k-1}) + \sigma(P_{n-2k-4})\sigma(P_{2k-2})]\sigma(P_{2k+1})\sigma(P_{n-2k-3})
\end{aligned}
$$

$$=\sigma^2(P_{2k})\sigma^2(P_{n-2k-4})$$
$$+[\sigma(P_{2k})\sigma(P_{2k+1})-\sigma(P_{2k-2})\sigma(P_{2k+1})]\sigma(P_{n-2k-3})\sigma(P_{n-2k-4})$$
$$-\sigma(P_{2k+1})\sigma(P_{2k-1})\sigma^2(P_{n-2k-3})$$
$$=\sigma^2(P_{2k})\sigma^2(P_{n-2k-4})+\sigma(P_{2k+1})\sigma(P_{2k-1})\sigma(P_{n-2k-3})\sigma(P_{n-2k-4})$$
$$-\sigma(P_{2k+1})\sigma(P_{2k-1})\sigma^2(P_{n-2k-3})$$
$$=\sigma^2(P_{2k})\sigma^2(P_{n-2k-4})-\sigma(P_{2k+1})\sigma(P_{2k-1})\sigma(P_{n-2k-3})\sigma(P_{n-2k-5})$$
$$=\sigma^2(P_{2k})\sigma^2(P_{n-2k-4})-\sigma(P_{2k+1})\sigma(P_{2k-1})\sigma(P_{n-2k-5})\sigma(P_{n-2k-4})$$
$$-\sigma(P_{2k+1})\sigma(P_{2k-1})\sigma^2(P_{n-2k-5})$$
$$=[\sigma(P_{2k})\sigma(P_{n-2k-4})+\sigma(P_{2k+1})\sigma(P_{n-2k-3})]\times$$
$$[\sigma(P_{2k})\sigma(P_{n-2k-4})-\sigma(P_{2k-1})\sigma(P_{n-2k-3})]$$
$$-[\sigma(P_{2k+1})\sigma(P_{2k-1})-\sigma^2(P_{2k})]\sigma(P_{n-2k-4})\sigma(P_{n-2k-5})$$
$$<0,$$
(*from Properties* 2 *and* 3),

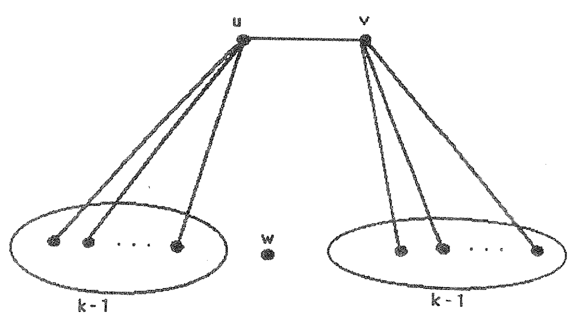
i.e., $\Delta_{uv}(C_n)<0$, for $d(u,v)=r+1=2k+2$ (*even*). Thus, the theorem is also true for $r=2k+1$.

The proof is now complete. □

From the equality that $\Delta_{uv}(G)=c(\overline{G-u})c(\overline{G-v})-c(\overline{G})c(\overline{G-u-v})$, we can show that the **Assertion** is true for $G=K_n-e$, $K_{m,n}$, $K_{m,n}-e$, $K_{n_1,n_2,\cdots,n_r}$, $K_n-E(C_r)$, $K_n-E(M_r)$, $K_{m,n}-E(C_r)$ and $K_{m,n}-E(M_r)$ etc., where e is an edge, C_r is the cycle with r vertices and M_r is an r-matching.

3. Counter Examples.

Let $n=2k+1$ and H be the graph shown in Figure 1.



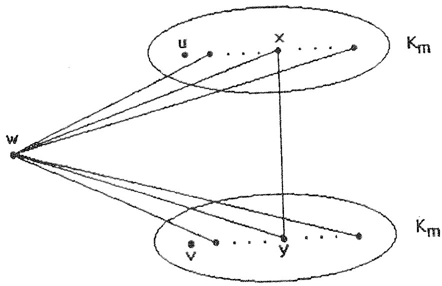
(Figure 1)

For $G = \overline{H}$, we have $d_G(u,v) = 2$. It is not difficult to see that

$$\Delta_{uv}(G) = k^2 - 2k \geq 0, \ if \ k \geq 2.$$

These examples show that the **Assertion** is not always true for $d(u,v)$ even. Obviously, examples can also be constructed from this idea for n even.

Let m be a positive integer and G be the graph shown in Figure 2.



(Figure 2)

Then, we have $d_G(u,v) = 3$. It is not difficult to see that

$$\Delta_{uv}(G) = -m^2 + 2m + 1 < 0, \ if \ m \geq 3.$$

These examples show that the **Assertion** is also not true for $d(u,v) = 3$ (odd).

4. Concluding Remark.

Since the **Assertion** for $\sigma(G)$ has many applications in chemistry, it is useful to single out those graphs for which the **Assertion** is true . We conjecture that it is true for unicyclic graphs.

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