Nullities of Unicyclic Graphs Revisited

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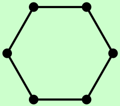
This is a joint work with Tsu-Hsien Huang (黃祖賢).

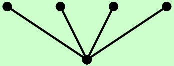
G: (simple, undirected) graph, with vertices $v_1, \ldots, v_n$

P_4 : 

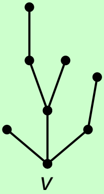
a path on 4 vertices

C_6 : 

a cycle on 6 vertices

S_5 : 

a star on 5 vertices



a rooted tree with root v and depth 3

$A(G)$: $(0,1)$-adjacency matrix of G ($v_i v_j \in E(G)$ iff $a_{ij} = 1$)

$\eta(G)$:= null($A(G)$) = dim $\mathcal{N}(A(G)) = \mathrm{alg\,mult}_{A(G)}(0)$,

$r(G)$:= rank(A(G)), *rank of G*

$$r(G) + \eta(G) = |V(G)|.$$

$$A(C_4) = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

Note that $r(C_4) = 2$, so $\eta(C_4) = 2$.

Lemma 1.

$$\eta(P_n) = \begin{cases} 1 & \text{if } n \text{ is odd} \\ 0 & \text{if } n \text{ is even} \end{cases}, \eta(C_n) = \begin{cases} 2 & \text{if } n|4 \\ 0 & \text{otherwise} \end{cases}.$$

L. Collatz and U. Sinogowitz (1957) first posed the problem of characterizing singular graphs.

Hückel molecular orbital theory (1931): If G is a bipartite graph that represents an alternant hydrocarbon and if $\eta(G) > 0$, then the chemical compound is unstable, or nonexistent.

L. Wang and D. Wong (2014) established the following:

Theorem A. For a graph G,

$$\lceil \frac{r(G)-c(G)}{2} \rceil \leq m(G) \leq \lfloor \frac{r(G)+2c(G)}{2} \rfloor.$$

$m(G)$: matching number of G, the size of a maximum matching.

(A *matching* in a graph is a set of pairwise non-adjacent edges.)

$c(G) := |E(G)| - |V(G)| + \theta(G)$, the *cyclomatic number* of G.

$\theta(G)$: the number of (connected) components of G.

For a connected graph G, $c(G) = 0$ iff G is a tree;

$c(G) = 1$ iff G has precisely one cycle.

A connected graph with precisely one cycle is called *unicyclic*.

[Can't have: $c(G) = 0$ and $r(G)$ odd.

When $c(G) = 0$, G is a forest. Then

$r(G) = |V(G)| - \eta(G) = |V(G)| - (|V(G)| - 2m(G)) = 2m(G)$.]

Theorem A'. For a graph G,

$$|V(G)| - 2m(G) - c(G) \leq \eta(G) \leq |V(G)| - 2m(G) + 2c(G).$$

2015, Ya-zhi Song, Xiao-qui Song (宋曉秋; China Univ. of Mining and Technology, Xuzhou) and B.-S. Tam: graphs attaining the upper bound

2016, Sa Rula, An Chang (常安; Fuzhou Univ.), Yirong Zheng; and also Long Wang (Anhui Univ. of Sci. Tech.): the lower bound

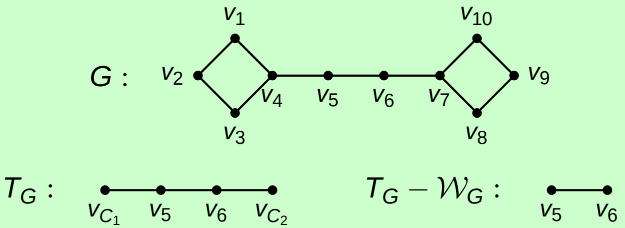
To describe the characterizations, more definitions are in order.

G: a graph with pairwise vertex-disjoint cycles.

T_G: the acyclic graph obtained from G by contracting cycles.

$V(T_G) := U \cup \mathcal{W}_G$, where U consists of vertices of G that do not lie on a cycle and $\mathcal{W}_G = \{v_C : C \text{ is a cycle of } G\}$.

Example 1.



$T_G - \mathcal{W}_G$: the graph obtained from T_G by deleting vertices in $\mathcal{W}_G$ and the incident edges.

Theorem B. For any graph G,

(i) (Song et.al., 2015) $\eta(G) = |V(G)| - 2m(G) + 2c(G)$ iff the following are satisfied:

(a) Distinct cycles of G (if any) are vertex-disjoint;

(b) The length of each cycle of G (if any) is a multiple of 4;

(c) $m(T_G) = m(T_G - \mathcal{W}_G)$ or, equivalently, there exists a maximum matching of T_G that does not saturate any vertex in $\mathcal{W}_G$.

(ii) (Rula et. al.; Wang, 2016) $\eta(G) = |V(G)| - 2m(G) - c(G)$ iff the following conditions are all satisfied: (a), (c) and

(b′) The length of each cycle of G (if any) is odd.

Proofs by induction on $c(G)$ and rely on earlier nontrivial results on unicyclic graphs due to J.-M. Guo, W.-G. Yan and Y.-N. Yeh (2009).

Guo et. al prove that if G is a unicyclic graph, then $\eta(G) = |V(G)| - 2m(G) - 1, |V(G)| - 2m(G)$ or $|V(G)| - 2m(G) + 2$.

They characterize each of these three types of unicyclic graphs, as well as nonsingular unicyclic graphs.

The Sachs theorem plays a key role in their proofs.

Guo et. al touch upon the concept of a canonical unicyclic graph G^* associated with a unicyclic graph G. However, the concept does not play a key role in their development, and it appears that there are many things not well understood, and some of the proofs are incomplete.

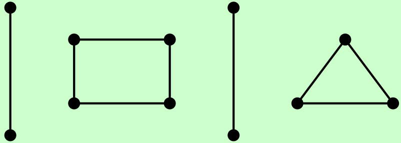
Theorem C (Sachs theorem). If $P_G(t) = t^n + a_1 t^{n-1} + \cdots + a_n$ is the characteristic polynomial of the graph G, then

$$a_i = \sum_U (-1)^{p(U)} 2^{c(U)}, i = 1, 2, \ldots, n,$$

where the sum is taken over all subgraphs U of G on i vertices that are disjoint union of K_2's and cycles (of order ≥ 3) (known as "elementary subgraphs").

An elementary subgraph on 11 vertices:

U :



$p(U) := \#$ of components $= 4$; $c(U) := \#$ of cycle components $= 2$.

Note that $P_G(t) = t^n + \sum_{i=1}^{k} a_i t^{n-i}$, where $n = |V(G)|$ and k is the size of the largest elementary subgraph in G; so $\eta(G) \geq n - k$. Hence, $\eta(G) \geq \#$ of vertices not covered by a largest elementary subgraph, and with equality if $(-1)^{p(U)}$ is the same for every largest elementary subgraph U.

For a tree T, we have $\eta(T) = |V(T)| - 2m(T)$, because every largest elementary subgraph of T is made up of $m(T)$ K_2s.

For a unicyclic graph G with cycle C_l, $l \equiv 2 \pmod 4$, we still have $\eta(G) = |V(G)| - 2m(G)$; but no longer so if $l \equiv 0 \pmod 4$.

Theorem D (Guo et. al). Let G be a unicyclic graph with cycle C_l.

(1) $\eta(G) = |V(G)| - 2m(G) - 1$ if $m(G) = \frac{l-1}{2} + m(G - C_l)$;

(2) $\eta(G) = |V(G)| - 2m(G) + 2$ if G has no maximum matching with an edge between $V(C_l)$ and $V(G - C_l)$, and $m(G) = \frac{l}{2} + m(G - C_l), l \equiv 0 \pmod{4}$;

(3) $\eta(G) = |V(G)| - 2m(G)$, otherwise.

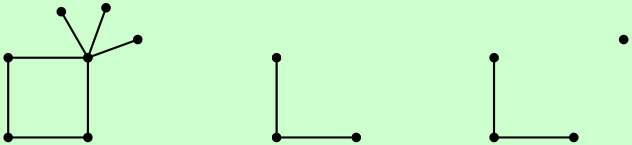
So, for a unicyclic graph G, $\eta(G)$ takes one of the following three values:

$|V(G)| - 2m(G) - 1, |V(G)| - 2m(G) + 2$ or $|V(G)| - 2m(G)$.

We will offer a short direct proof for the latter fact.

Pendant vertex : a vertex of degree one.

A vertex-induced subgraph H of G is a *pendant star* of G if H is a star such that all pendant vertices of H are also pendant vertices in G.



G with a pendant S_4 $\quad$ $G - S_4$ $\quad$ $G - S_3$

Lemma 2. Let G be a graph with pendant vertex u, and let v be the neighbor of u in G. Then $\eta(G) = \eta(G - u - v)$.

Proof. For brevity, denote $G - u - v$ by H. We may assume that

$$A(G) = \begin{array}{c} \\ u \\ v \\ \\ \\ \\ \end{array} \begin{array}{c} \begin{array}{cc} u & v \end{array} \\ \left[\begin{array}{cc|ccc} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & & y^T & \\ \hline 0 & & & & \\ \vdots & y & & A(H) & \\ 0 & & & & \end{array}\right] \end{array}$$

If $x \in \mathcal{N}(A(G))$ then $x_v = 0$, $x_u = -y^T x[V(H)]$ and $x[V(H)] \in \mathcal{N}(A(H))$. The converse is also true.

Take a basis $\{z^{(1)}, \ldots, z^{(k)}\}$ for $\mathcal{N}(A(H))$, and for $i = 1, \ldots, k$, let $x^{(i)}$ denote the vector in $\mathbb{R}^{|V(G)|}$ such that $x^{(i)}[V(H)] = z^{(i)}$, $(x^{(i)})_v = 0$ and $x_u^{(i)} = -y^T z^{(i)}$. Then $\{x^{(1)}, \ldots, x^{(k)}\}$ is a basis for $\mathcal{N}(A(G))$. Hence, we obtain $\eta(H) = \eta(G)$, as desired. ∎

Corollary 1. If S_k is a pendant star of G, then

$$\eta(G) = \eta(G - S_k) + (k - 2).$$

Proof. Observe that if v is the star center of S_k and u is one of the pendant vertices in S_k, then $G - u - v = (G - S_k) \cup (k - 2)K_1$. ∎

Lemma 3. If S is a pendant star of G, then $m(G) = m(G - S) + 1$.

Proof. We have $m(G) \geq m(G - S) + m(S) = m(G - S) + 1$. To show the reverse inequality, let M be a maximum matching for G. Note that M must saturate the star center of S. Furthermore, we may assume that the edge of M that saturates the star center is a pendant edge of S. So we have $M \subset (M \cap E(G - S)) \cup (M \cap E(S))$, and hence the reverse inequality. ■

Lemma 4. If S is a pendant star of G, then

$\eta(G - S_k) - |V(G - S_k)| + 2m(G - S_k) = \eta(G) - |V(G)| + 2m(G)$.

[The inequalities for bounds of $\eta(G)$ can be rewritten as:

$$-c(G) \leq \eta(G) - |V(G)| + 2m(G) \leq 2c(G).]$$

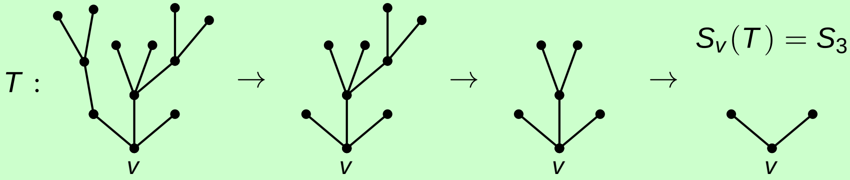
A *canonical unicyclic graph* is a cycle together with pendant stars attached at none, some or all of its vertices.

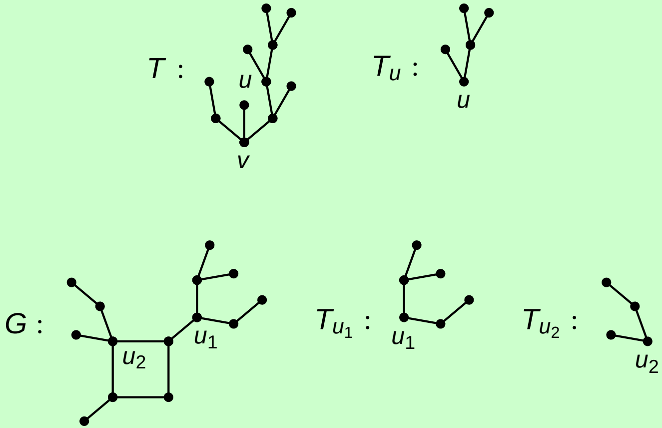
Quote from Guo et. al.:

"If G (unicyclic) is not canonical, G contains at least one pendant star H_1 such that $G - H_1$ is also a unicyclic graph. We call the procedure of obtaining $G - H_1$ from G a ‘deleting opertor’. With repeated applications of the ‘deleting operators’, then a canonical unicyclic graph, denoted by G^*, is obtained from G."

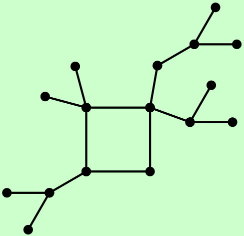
The uniqueness of G^* wasn’t considered. I’ll consider the ‘deleting operator’ for a rooted tree first.

Let T be a rooted tree with root v. Suppose that T is not the single vertex graph K_1, nor a star with star center v. Then T must have a pendant star S such that $T - S$ is a tree containing vertex v. Repeating the process, one ends up with either a K_1 (at v) or a star with star center v. We denote it by $S_v(T)$.

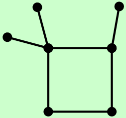




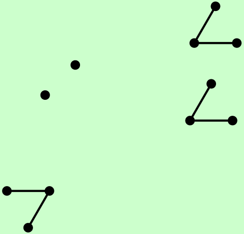
The canonical unicyclic graph G^* associated with a unicyclic graph G is obtained from G by replacing T_v by $S_v(T_v)$ for every vertex v in the cycle of G.



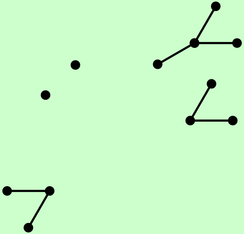
A unicyclic garph G



G^*, the canonical unicyclic graph associated with G



$G - G^*$



$G - C$

From the above, for a unicyclic graph G, we have

$\eta(G) - |V(G)| + 2m(G) = \eta(G^*) - |V(G^*)| + 2m(G^*)$.

Now G^* is either an odd cycle, an even cycle, or a canonical unicyclic graph, different from a cycle. In each case, we can compute $\eta(G^*) - |V(G^*)| + 2m(G^*)$. So we readily obtain

Theorem E (cf. Guo et. al, Cor. 2.1). Let G be a unicyclic graph with cycle C_l. Then

$$\eta(G) - |V(G)| + 2m(G) = \begin{cases} -1 & \text{if } G^* = C_l \text{ with } l \text{ odd} \\ 2 & \text{if } G^* = C_l \text{ with } l \equiv 0 \pmod 4 \\ 0 & \text{otherwise} \end{cases}.$$

By the preceding theorem, if G is a unicyclic graph, then

$|V(G)| - 2m(G) - 1, |V(G)| - 2m(G) + 2$ and $|V(G)| - 2m(G)$ are the three possible values for $\eta(G)$.

In Guo et.al, it is said that Theorem E can be obtained from its Theorem 2.1 (i.e, Theorem D) and its Theorem 2.2, which essentially is equivalent to the fact that

$\eta(G) - |V(G)| + 2m(G) = \eta(G^*) - |V(G^*)| + 2m(G^*)$, [as well as Lemma 2.4 (i.e., Lemma 3)].

[Recall **Theorem D**. Let G be a unicyclic graph with cycle C_l. Then:

(1) $\eta(G) = |V(G)| - 2m(G) - 1$ if $m(G) = \frac{l-1}{2} + m(G - C_l)$;]

Exploiting the concept of G^*, we can offer a conceptual proof for a strengthened combined form of Theorem D and Theorem E.

Theoem F. Let G be a unicyclic graph with cycle C_l.

(i) $\eta(G) = |V(G)| - 2m(G) - 1$ if and only if

$m(G) = \frac{l-1}{2} + m(G - C_l)$ if and only if $G^* = C_l$ and l is odd.

(ii) $\eta(G) = |V(G)| - 2m(G) + 2$

$\Leftrightarrow l \equiv 0 (\mathrm{mod}\ 4)$ and G does not have a maximum matching with an edge between$V(C_l)$ and $V(G - C_l)$

$\Leftrightarrow m(G) = \frac{l}{2} + m(G - C_l), l \equiv 0 (\mathrm{mod}\ 4)$ and G does not have a maximum matching with an edge between $V(C_l)$ and $V(G - C_l)$

$\Leftrightarrow G^* = C_l$ and $l \equiv 0 \pmod 4$.

(iii) $\eta(G) = |V(G)| - 2m(G)$ if and only if otherwise.

Lemma 5. Let T be a tree and let v be a vertex of T. Then:

(i) The following conditions are equivalent:

  (a) $S_v(T) = K_1$.

  (b) For each $u \in N(v)$, $S_u(T_u)$ is a star.

  (c) T has a maximum matching that does not saturate vertex v.

  (d) $m(T) = m(T - v)$.

(ii) The following conditions are equivalent:

  (a) $S_v(T)$ is a star.

  (d) $m(T) = m(T - v) + 1$.

Lemma 6. Let G be a graph obtained from vertex-disjoint graphs G_1 and G_2 by identifying a vertex in G_1 and a vertex in G_2 as the vertex v of G. Suppose that $m(G_2) = m(G_2 - v)$. Then:

(a) $m(G) = m(G_1) + m(G - G_1)$.

(b) G has a perfect matching iff G_1 and $G - G_1$ both have perfect matchings, and every perfect matching of G (if any) is the union of a perfect matching of G_1 and a perfect matching of G_2.

Lemma 7. For a unicyclic graph G with cycle C_l, the following hold:

(1) $m(G) = m(G^*) + m(G - G^*)$;

(2) $m(G - G^*) = m(G - C_l)$;

(3) every maximum matching of G does not have an edge between $V(C_l)$ and $V(G - C_l)$ iff $G^* = C_l$ with l even or $G = C_l$.

Lemma 8. For a unicyclic graph G, G is nonsingular iff G^* and $G - G^*$ are both nonsingular.

Theorem 1. Let G be a unicyclic graph with cycle C_l. Then G is nonsingular if and only if either $G^* = C_l$ with $l \not\equiv 0 \pmod 4$ and $G - C_l$ has a perfect matching, or G has a unique perfect matching.

Corollary 2 (Guo, et.al. Theorem 3.4). Let G be a unicyclic graph with cycle C_l. Then G is nonsingular if and only if one of the following (mutually exclusive) conditions is satisfied:

(1) l is odd and $G - C_l$ contains a perfect matching.

(2) G contains a unique perfect matching.

(3) $l \not\equiv 0 \pmod 4$ and G has precisely two perfect matchings.

The proof for the above Corollary 2 as given in Guo et.al. is incomplete.

The following not entirely obvious facts are used, without proof:

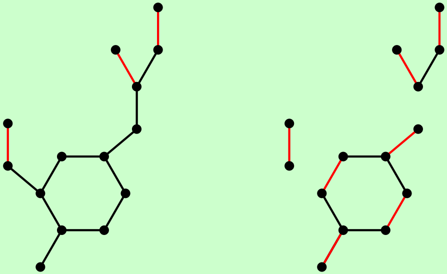
(1) If G has a perfect matching, then G has at most two perfect matchings.

(2) If an odd-unicyclic graph has a perfect matching, then its perfect matching is unique.

(3) If G contains two perfect matchings, then $G - C_l$ has a (unique) perfect matching.

Suppose G has a perfect matchng.

1° $G^* \neq C_l$: Then G^* must have pendant stars and, moreover, upon removing a pendant edge, the resulting graph is necessarily a union of even paths. It follows that G^*, and hence G, must have a unique perfect matching.



A unicyclic graph G $\qquad$ G^* and $G - G^*$

[If a tree (or, more generally, a forest) has a perfect matching, its perfect matching is unique.]

[It can be proved that G has a perfect matching iff G^* and $G - G^*$ both have perfect matchings and, moreover, every perfect matching of G is the union of a perfect matching of G^* and a perfect matching of $G - G^*$.]

2° $G^* = C_l$

(i) If l is even, then $G^* = C_l$, and hence G, has precisely two perfect matchings.

(ii) If l is odd, then G^*, and hence G, has no perfect matchings, contradiction.

(1), (2) and (3) now follow.

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