Characterization of Graphs with Large Nullity

束金龙 翟清明

华东师范大学
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1. Definition

Let $A(G)$ be the adjacent matrix of graph $G$. The set of all eigenvalues of $A(G)$ including multiplicity is called the spectrum of $G$. The nullity of a graph $G$, denoted by $\eta(G)$, is the multiplicity of the eigenvalue zero in its spectrum.
2. Background

In [3], L.Collatz and U.Sinogowitz first posed the problem of characterizing all graphs with $\eta(G) > 0$. This question is of great interest in chemistry, because, as has been known in [4], for a bipartite graph $G$ (corresponding to an alternate hydrocarbon), if $\eta(G) > 0$, then it indicates that the molecule which such a graph represents is unstable. The question is of interest also for non-bipartite graphs (corresponding to non-alternate hydrocarbons), but a direct connection with chemical stability is in these cases not so straightforward.

\[ \eta = 0 \quad \eta = 1 \quad \eta = 2 \]
3. Problem

(i) The nullity of some classes of graphs, such as bipartite graphs, trees, unicyclic graphs, bicyclic graphs, and so on.

(ii) Graphs with small nullity, such as nonsingular (i.e. $\eta = 0$) graphs and quasi-nonsingular graphs (see [2],[8-9],[11],[18]).

(iii) Graphs with large nullity (see [1-2],[10],[16-17],[19]).
4. Nullity on Bipartite Graphs

By the definition, we have

Proposition 4.1 \( \eta(G) = n - \text{rank}(A(G)) \) for any graph \( G \).

Specially, for bipartite graph \( G \) with

\[
A(G) = \begin{pmatrix} O & B \\ B^T & O \end{pmatrix},
\]

we have the following corollaries.

Corollary 4.2 \( \eta(G) = n - 2\text{rank}(B) \).

Corollary 4.3 Let \( G = (V_1, V_2, E) \), with \( |V_2| \geq |V_1| \), be a bipartite graph. Then if \( \eta(G) \geq |V_2| - |V_1| \), with equality if and only \( \text{rank}(B) = |V_1| \).
The following results enable, in special cases, the reduction of the problem of determining $\eta(G')$ for some graphs to the same problem for simpler graphs.

**Theorem 4.4 (D.Cvetković, I.Gutman, [7])**

[The algebraic multiplicity of the number zero in the spectrum of a bipartite graph, Mat.Vesnik 9(1972) 141-150.]

Let $G_1 = (V_1, V'_1, E_1)$ and $G_2 = (V_2, V'_2, E_2)$ be two bipartite graphs, where $\eta(G_1) = |V'_1| - |V_1|$. If the graph $G$ is obtained from $G_1$ and $G_2$ by arbitrarily joining vertices from $V_1$ to vertices in $V_2$ (or $V'_2$), then $\eta(G) = \eta(G_1) + \eta(G_2)$. 
Corollary 4.5 If the bipartite graph $G$ contains a pendant vertex $u$, which is adjacent to $v$, then $\eta(G') = \eta(G - u - v)$.

Corollary 4.6 Let $G_1$ and $G_2$ be bipartite graphs. If $\eta(G_1) = 0$, and if the graph $G$ is obtained by joining a vertex of $G_1$ by an edge with a vertex of $G_2$, then $\eta(G') = \eta(G_2)$. 
Theorem 4.7 (D. Cvetković, I. Gutman, N. Trinajstić, [12])
[Graph theory and molecular orbitals, II. Croat. Chem. Acta 44(1972)365-374.]
A path with four vertices of degree 2 in a bipartite graph $G$ can be replaced by an edge without changing the value of $\eta(G)$ (see Fig.1).

Theorem 4.8 (D. Cvetković, I. Gutman, N. Trinajstić, [12])
[Graph theory and molecular orbitals, II. Croat. Chem. Acta 44(1972)365-374.]
Two vertices and the four edges of a cycle of length 4, which are positioned in a bipartite graph $G'$, can be removed without changing the value of $\eta(G')$ (see Fig.2).

![Fig.1](image1)

![Fig.2](image2)
Remark 4.9 (I.Gutman, N.Trinajstić, [13])

[Graph theory and molecular orbitals, XV. The Hückel rule. J.Chem.Phys. 64(1976)4921-4925.]

Corollary 4.5, Theorem 4.7 and 4.8 hold also in the case when $G$ is not a bipartite graph.
**Theorem 4.10 (H.C.Longuet-Higgins, [4])**


If $G$ is a connected bipartite graph with $\eta(G) = 0$, then $G$ has a 1-factor.

**Theorem 4.11 (D.Cvetković, I.Gutman, N.Trinajstić, [12])**

[Graph theory and molecular orbitals, II. Croat, Chem. Acta 44(1972)365-374.]

If a bipartite graph $G$ does not contain any cycles of lengths $4s$ ($s = 1, 2, \cdots$), then $\eta(G) = n - 2m(G)$, where $m(G)$ is the size of maximum matching in $G$. 
5. Tree, Unicyclic Graph and Bicyclic Graph

The following is a direct result of Theorem 4.11.

**Theorem 5.1 (D. Cvetković, I. Gutman, [7])**

[The algebraic multiplicity of the number zero in the spectrum of a bipartite graph, Mat. Vesnik 9(1972) 141-150.]

For any tree $T$, $\eta(T) = n - 2m(T)$. 
Denote by $\mathcal{T}(n, D)$ the set of all $n$-vertex trees in which all vertex degrees are less than or equal to $D$, where $D$ is a positive integer. Furthermore, let $\mathcal{T}(D) = \bigcup_{n \geq 1} \mathcal{T}(n, D)$. $D \leq 2$ is trivial.

**Theorem 5.2 (S. Fiorini, I. Gutman, I. Sciriha, [10])**

[Trees with maximum nullity, Linear Algebra Appl. 397(2005) 245-251.]

For all $n \geq 1$ and $D \geq 3$, if $T \in \mathcal{T}(n, D)$, then $\eta(T) \leq n - 2\lceil (n - 1)/D \rceil$. For all $n \geq 1$ and $D \geq 3$, there exist trees $T \in \mathcal{T}(n, D)$ such that $\eta(T) = n - 2\lceil (n - 1)/D \rceil$.

In [10], S. Fiorini etc. also investigate trees with maximal nullity and present a conjecture that characterizes all trees with $\eta(T) = n - 2\lceil (n - 1)/D \rceil$. 

Let $C_n$ be the cycle of order $n$. Since the spectrum of $C_n$ is 
$\{2 \cos \frac{2\pi r}{n} | r = 0, 1, \cdots, n - 1\}$, we have

**Proposition 5.3**

If $n \equiv 0 \pmod{4}$, then $\eta(C_n) = 2$; otherwise, $\eta(C_n) = 0$.

**Theorem 5.4 (X.Z.Tan, B.L.Liu, [2])**


Let $\mathcal{U}_n$ be the set of unicyclic graphs with $n$ vertices. The nullity set of $\mathcal{U}_n$ ($n \geq 5$) is $\{0, 1, \cdots, n - 4\}$. 
Definition 5.5

A unicyclic graph $U$ is called \textit{elementary unicyclic graph} if

(i) $U$ is a cycle whose length can not be divided by 4, or,

(ii) let $t$ be an integer satisfying $0 < t \leq l$, and $l \equiv t \pmod{2}$. $U$ is obtained from $C_l$ and $tK_1$ by the rule: First select $t$ vertices from $C_l$ such that there are an even number (which may be 0) of vertices between any two consecutive such vertices. Then join an edge from each of the $t$ vertices to an isolated vertex.
The following two theorems investigate the unicyclic graphs with extremal nullity, i.e., the unicyclic graphs satisfying $\eta(U) = 0$ or $\eta(U) = n - 4$. [2] shows that the condition in Theorem 5.6 is sufficient and [14] shows that the condition is necessary.

**Theorem 5.6 (X.Z.Tan, B.L.Liu, [2]; C.Y.Song, Q.X.Huang, [14])**


Let $U \in \mathcal{U}_n$. Then $\eta(U) = 0$ if and only if $U$ is an elementary unicyclic graph or a graph obtained by joining a vertex of PM-trees with an arbitrary vertex of an elementary unicyclic graph, where PM-tree refers to a tree with perfect matching.
Theorem 5.7 (X.Z. Tan, B.L. Liu, [2])


Let $U \in \mathcal{U}_n (n \geq 5)$. Then $\eta(U) = n - 4$ if and only if $U$ is isomorphic to one of the following graphs.
Theorem 5.1 shows that $\eta(T) = n - 2m(T)$ for any tree $T$. The following finds the connection between $\eta(U)$ and $m(U)$ for unicyclic graph $U$.

**Theorem 5.8 (C.Song, Q.Huang, [14]; J.Guo, W.Yan, Y.N, Yeh, [15])**

[The nullity of unicyclic graphs, submitted.]
[On the nullity and the matching number of unicyclic graphs, submitted.]

Let $U \in \mathcal{U}_n$. Then $\eta(U) = n - 2m(U) - 1$ or $n - 2m(U)$ or $n - 2m(U) + 2$. Moreover, the three classes of unicyclic graphs are completely determined.
Bicyclic graphs have some similar results with unicyclic graphs.

**Theorem 5.9 (S.B.Hu, B.L.Liu, X.Z.Tan, [16]; X.Yuan, H.Shan, Y.Liu, [17])**

[The nullity set of bicyclic graphs, J. Tongji University, To appear (in Chinese).]

Let $\mathcal{B}_n$ be the set of bicyclic graphs with $n$ vertices. The nullity set of $\mathcal{B}_n$ ($n \geq 6$) is $\{0, 1, \cdots, n - 4\}$. 
Theorem 5.10 (S.B.Hu, B.L.Liu, X.Z.Tan, [16]; X.Yuan, H.Shan, Y.Liu, [17])

[The nullity set of bicyclic graphs, J. Tongji University, To appear (in Chinese).]

Let \( B \in \mathcal{B}_n \). Then \( \eta(B) = n - 4 \) if and only if \( B \) is isomorphic to one of the following graphs.

![Graphs](image-url)
6. Graphs with small nullity

Theorem 6.1 (I.Sciriha, I.Gutman, [9])
Let $T$ be a tree, then its line graph $L(T)$ is either non-singular (i.e. $\eta(L(T)) = 0$) or has nullity one.
Q.X. Huang and J.X. Meng extend the above result to a more general class of graphs. A connected graph $G$ is said to be quasi-nonsingular if it is a nonsingular block or there exist a cut vertex $u$ and a component $H$ of $G - u$ such that $\eta(H) + \eta(G - V(H)) \leq 1$.

**Theorem 6.2 (Q.X. Huang, J.X. Meng, [18])**

[The nullity of quasi-nonsingular graph, Discrete Math. To appear.]

A quasi-nonsingular graph has nullity at most 1.
A block-complete graph is a connected graph whose blocks are all complete graphs. A block-complete graph is said to be proper if each cut vertex lies in at most two $K_2$-blocks (other blocks containing the cut vertex are not $K_2$’s). The line graphs of trees consist of a subclass of proper-block-complete graphs. The following theorem indicates that the line graph of a tree is also a quasi-nonsingular graph. And hence Theorem 6.2 contains the result of Theorem 6.1.

Theorem 6.3 (Q.X.Huang, J.X.Meng, [18])
[The nullity of quasi-nonsingular graph, Discrete Math. To appear.]
Let $G$ be a proper-block-complete graph. Then $G$ is quasi-nonsingular graph.
7. Graphs with large nullity

Theorem 5.7 and 5.10 have characterized unicyclic graphs and bicyclic graphs with nullity $n - 4$, respectively. This section investigates general graphs with large nullity.

Theorem 7.1 (B.Cheng, B.L.Liu, [2]; X.Yuan, H.Shan, Y.Liu, [17])


Let $G$ be a graph with $n$ vertices. Then
(i) $\eta(G) = n - 2$ if and only if $G \cong K_{a,b} \cup (n - a - b)K_1$;
(ii) $\eta(G) = n - 3$ if and only if $G \cong K_{a,b,c} \cup (n - a - b - c)K_1$. 
We continue the study of Theorem 5.7, 5.10 and 7.1 on graphs with large nullity.

Lemma 7.2 (I. Gutman, N. Trinajstić, [13])

[Graph theory and molecular orbitals, XV. The Hückel rule. J.Chem.Phys. 64(1976)4921-4925.]

Let \( u \) be a pendant vertex of \( G \) and \( v \) be its neighbor, then \( \eta(G - u - v) = \eta(G) \).

Lemma 7.3

For any vertex \( v \) of graph \( G \), \( \eta(G) - 1 \leq \eta(G - v) \leq \eta(G) + 1 \).

Proof  It is a direct result of the well-known Interlacing Theorem. □
Definition 7.4

For given positive integers \( \delta \) and \( n \), we now define two classes of graphs with minimum degree \( \delta \) and order \( n \). Let \( \mathcal{G}_1(n, \delta) \) be the set of graphs obtained from a complete bipartite graph \( K_{n-\delta, \delta} \) by adding at least an edge in \( V_\delta \) (where \( V_\delta \) refers to the partition set with \( \delta \) vertices) and \( \mathcal{G}_2(n, \delta) \) be the set of graphs obtained from two complete bipartite graphs \( K_{a,b} \) and \( K_{c,\delta} \) by adding some (possibly, 0) edges from \( V_\delta \) to \( V_a, V_b \) and \( V_\delta \), where \( a + b + c + \delta = n \).
Theorem 7.5 Let $G$ be a graph with $\eta(G) = n - 4$ and $\delta \geq 1$, then $G \in G_1(n, \delta) \cup G_2(n, \delta)$.

Proof Let $u \in V(G)$ with $d_G(u) = \delta$, $N_G(u) = \{v_1, v_2, \cdots, v_\delta\}$ and $H \cong G - \{v_i | i = 1, 2, \cdots, \delta - 1\}$. By Lemma 7.3, $\eta(H) \geq \eta(G) - (\delta - 1) = n(H) - 4$. On the other hand, clearly $\eta(H) \leq n(H)$. Since $H$ has at least an edge $uv_\delta$, $\eta(H) \neq n(H)$. Thus $n(H) - 4 \leq \eta(H) \leq n(H) - 2$.

Assume that $\eta(H) = n(H) - 3$. Since $uv_\delta$ is a pendant edge of $H$, $\eta(H - u - v_\delta) = \eta(H)$ by Lemma 7.2. This implies that $\eta(H - u - v_\delta) = n(H - u - v_\delta) - 1$, which is impossible. Next we only need consider the following two cases.
Case 1. $\eta(H) = n(H) - 2$.

Now, $\eta(H - u - v_\delta) = n(H - u - v_\delta)$ and hence $H - u - v_\delta$ is an empty graph. This implies that $N_G(x) = N_G(u) = \{v_1, v_2, \cdots, v_\delta\}$ for any $x \in V(H - u - v_\delta)$. Moreover, there is at least an edge joining two neighbors of $u$, otherwise, $G \cong K_{n-\delta,\delta}$ and $\eta(G) = \eta(K_{n-\delta,\delta}) = n - 2$ by Theorem 7.1, which contradicts $\eta(G) = n - 4$. Thus $G \in \mathcal{G}_1(n, \delta)$.

Case 2. $\eta(H) = n(H) - 4$.

Now, $\eta(H - u - v_\delta) = n(H - u - v_\delta) - 2$ and hence $H - u - v_\delta$ is the union of a complete bipartite graph $K_{a,b}$ and some isolated vertices. And $N_G(x) = N_G(u) = \{v_1, v_2, \cdots, v_\delta\}$ for each isolated vertex $x$ of $H - u - v_\delta$. This implies that $G \in \mathcal{G}_2(n, \delta)$. □
Corollary 7.6

For any graph $G$ with $\delta = 1$, $\eta(G) = n - 4$ if and only if $G \in \mathcal{G}_2(n, 1)$.

Proof  We first show the necessity. Since $\eta(G) = n-4$, $G \in \mathcal{G}_1(n, 1) \cup \mathcal{G}_2(n, 1)$. Note that the definition of $\mathcal{G}_1(n, \delta)$ implies that $\delta \geq 2$. Thus $G \in \mathcal{G}_2(n, 1)$.

Conversely, if $G \in \mathcal{G}_2(n, 1)$, then $G$ is a graph obtained from $K_{a,b}$ and $K_{c,\delta}$ by adding edges from $V_\delta$ to $V_a$ and $V_b$. Let $V_\delta = \{u\}$ and $v \in V_c$. Then $G - u - v \cong K_{a,b} \cup (c - 1)K_1$ and hence $\eta(G - u - v) = n(G - u - v) - 2$. Since $uv$ is a pendant edge of $G$, $\eta(G) = \eta(G - u - v) = n(G - u - v) - 2 = n - 4$. $\square$
Corollary 7.7

(i) For any tree $T$, $\eta(T) = n - 4$ if and only if $T$ is $T_1$ or $T_2$.

(ii) ([2]) For any unicyclic graph $U$, $\eta(U) = n - 4$ if and only if $U$ is isomorphic to one of the following graphs.

![Graphs](image://graph.png)
Let $G$ be a bipartite graph with $\delta \geq 1$. Since $\eta(G) = n - 2\text{rank}(B)$, we immediately conclude that $\eta(G) \notin \{n - 1, n - 3\}$. By Theorem 6.1, $\eta(G) = n - 2$ if and only if $G$ is a complete bipartite graph. The following theorem characterizes bipartite graphs with nullity $n - 4$.

**Theorem 7.8**

Let $G$ be a bipartite graph with $\delta \geq 1$, then $\eta(G) = n - 4$ if and only if $G$ is obtained from $K_{a,b} \cup K_{c,d}$ by joining $V_b$ with a subset of $V_d$ (or joining $V_d$ with a subset of $V_b$), where $a + b + c + d = n$. 
A graph is said to be chordal, if every cycle of length greater than three has a chord, which is an edge joining two non-consecutive vertices of the cycle. Let $G$ be a chordal graph with $\delta \geq 1$. Then $G$ contains no induced subgraph $K_{2,2}$. By Theorem 6.1, $\eta(G) = n - 2$ if and only if $G$ is a star $K_{1,n-1}$ (i.e. $K_1 \nabla (n-1)K_1$). And $\eta(G) = n - 3$ if and only if $G \cong K_{1,1,n-2}$ (i.e. $K_2 \nabla (n-2)K_1$). The following theorem characterizes chordal graphs with nullity $n - 4$. 
Theorem 7.9

Let $G$ be a chordal graph with $\delta \geq 1$, then $\eta(G) = n - 4$ if and only if $G$ is isomorphic to $K_3 \nabla (n - 3)K_1$ or $G_i$ ($i = 1, 2, 3$).

(Dotted lines in $G_3$ mean that corresponding vertices are adjacent or not)
References


Thank you!