

Unicyclic Graphs with Nullity One

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Abstract The nullity of a graph G is defined to be the multiplicity of the eigenvalue zero in its spectrum. In this paper we characterize the unicyclic graphs with nullity one in aspect of its graphical construction.

Keywords nullity of graphs; unicyclic graphs; singularity; perfectly matched vertex.

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1. Introduction

Let G be a simple graph of order n with vertex set $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G)$. The adjacency matrix of G is a matrix $A = A(G) = [a_{ij}]$ of order n given by $a_{ij} = 1$ if v_i is adjacent to v_j , and $a_{ij} = 0$ otherwise. The nullity of the graph G is the multiplicity of the eigenvalue zero in the spectrum of $A(G)$, denoted by $\eta(G)$. When $\eta(G)=0$, the graph G is called nonsingular. In 1957, Collatz and Sinogowitz [1] first proposed the problem of characterizing all graphs G with $\eta(G) > 0$. This problem is of great interest in both chemistry and mathematics. For a bipartite graph G which corresponds to an alternant hydrocarbon in chemistry, if $\eta(G) > 0$, it is indicated that the corresponding molecule is unstable. The nullity of a graph is also meaningful in mathematics since it is related to the singularity of adjacent matrix. The problem has not yet been solved completely. Much attention is focused on graphs with few edges, e.g. trees, unicyclic graphs, bicyclic graphs.

The nullity of a tree can be given in explicit form in terms of the matching number of the tree [10]. Tan and Liu [6] gave the nullity set of unicyclic graphs on n vertices for $n \geq 5$, that is $\{0, 1, 2, \dots, n-4\}$. In addition, the unicyclic graphs with maximum nullity is characterized. For the unicyclic graphs with minimum nullity (or the singular unicyclic graphs), they proposed an open problem, which was at last solved by Li and Chang [7]. Hu, Liu and Tan [9] gave the nullity set of bicyclic graphs on n vertices for $n \geq 6$, that is, $\{0, 1, 2, \dots, n-4\}$, and characterized the bicyclic graphs with extremal nullity. In addition, in paper [8], the authors presented another version of characterization for an acyclic (respectively, a unicyclic graph) to be nonsingular. Other work on nullity of graphs can be found in [4] which proved that the nullity of the line

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graph of a tree is at most one, and in [3] which provided a method of constructing singular graphs from others of smaller order, and in [2] for related topics. Cheng and Liu [5] considered general graphs on fixed number of vertices with extreme nullity, and also discussed the maximal nullity of graphs with fixed number of vertices and edges.

We notice that in the paper [3] the author considered the graphs with nullity one. In this paper we focus on the problem of characterizing the unicyclic graphs with nullity one, and give the result in aspect of the graphical construction.

2. Preliminaries

In this section, we will first give some definitions and notations, then introduce some useful results on the nullity of graphs.

Let $G = (V, E)$ be a simple graph with vertex set $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G) = \{e_1, e_2, \dots, e_m\}$. Denote by $v(G)$ and $e(G)$ the number of vertices and edges of G . For any $v \in V$, denote by $d_G(v)$ and $N_G(v)$, respectively, the degree and neighborhood of v in G . A vertex $v \in V$ is called pendent if $d_G(v) = 1$, and a vertex $w \in V$ is called quasi-pendent if w is adjacent to a pendent vertex. Let W be a nonempty subset of $V(G)$. Denote by $G - W$ the graph obtained from G by removing the vertices of W together with all edges incident to them. Let F be a nonempty subset of $E(G)$. Denote by $G - F$ the graph obtained from G by removing the edges of F .

A matching of G is a collection of independent edges of G . A maximal matching is a matching with maximum possible number of edges, whose cardinality is called the matching number of G and is denoted by $m(G)$. If $m(G) = v(G)/2$, then G is said to have perfect matchings, or G is called a PM-graph for short. An edge belonging to a matching of a graph G is said to match its two end-vertices. A vertex v is said to be perfectly matched if it is matched by all maximal matchings of G , otherwise, v is called mismatched; see Figure 1.

It is easy to see that each quasi-pendent vertex must be perfectly matched, and if uv is a pendent edge of G , then there exists a maximal matching of G which contains it. Furthermore, if w is a mismatched vertex of G , then we can get a maximal matching of G which contains uv and w is mismatched in it. For a PM-tree T , let $u \in V(T)$ and $M(T)$ be one of its perfect matchings and $N_T(u) = \{v_1, v_2, \dots, v_m\}$. Without loss of generality, suppose v_1 is matched by $M(T)$, then each component of $T - u - v_1$ is still a PM-tree.

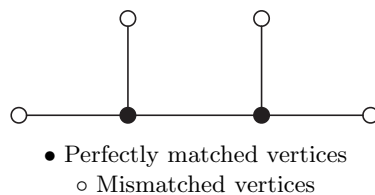


Figure 1 Perfectly matched and mismatched vertices

The disjoint union of k copies of a graph G is written by kG . A graph is called null if it has no edges. As usual, the cycle and the path of order n are denoted by C_n and P_n , respectively.

An isolated vertex is sometimes denoted by K_1 . A unicyclic graph is a simple connected graph with equal number of vertices and edges. Obviously, a unicyclic graph contains a unique cycle.

Lemma 2.1 ([2]) *For a graph G containing a pendent vertex, if the induced subgraph H is obtained by deleting this vertex together with the vertex adjacent to it, then $\eta(H) = \eta(G)$.*

By Lemma 2.1, we can get $\eta(P_n) = 1$ if n is odd and $\eta(P_n) = 0$ otherwise.

Lemma 2.2 ([2]) *Let $G = G_1 \cup G_2 \cup \cdots \cup G_n$, where G_1, G_2, \dots, G_n are disjoint connected components of G . Then*

$$\eta(G) = \sum_{i=1}^n \eta(G_i).$$

Lemma 2.3 ([2]) *A path with four vertices of degree 2 in a graph G can be replaced by an edge (see Figure 2) without changing the value of $\eta(G)$.*

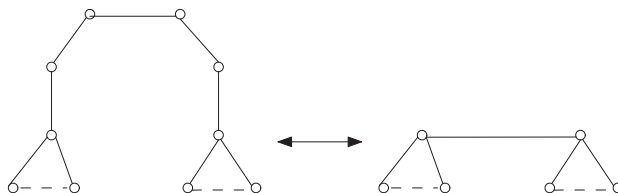


Figure 2 Illustration of Lemma 2.3

Consequently, by Lemma 2.3, if $n \equiv 0 \pmod{4}$, then $\eta(C_n) = 2$; otherwise, $\eta(C_n) = 0$.

Theorem 2.4 ([2]) *If T is a tree of order n , then $\eta(T) = n - 2m(T)$. Hence, $\eta(T) = 0$ if and only if T is a PM-tree.*

Lemma 2.5 *Let G be a connected graph obtained from a connected graph (possibly being K_1) by attaching at a vertex u a tree T (i.e., identifying the vertex u with some vertex of T). Then*

- (i) *If u is a perfectly matched vertex of T , $\eta(G) = \eta(G - T) + \eta(T)$;*
- (ii) *If u is a mismatched vertex of T , $\eta(G) = \eta(T - u) + \eta(G - (T - u))$.*

Proof (i) Using induction principle on $e(T)$. If $e(T) = 1$, then $T = P_2$ and u is a quasi-pendent vertex of G . By Lemma 2.1, $\eta(G) = \eta(G - T) + 0 = \eta(G - T) + \eta(T)$. Suppose the result holds for all trees T with $e(T) < m$. Now we consider the case of $e(T) = m$. If u is a unique quasi-pendent vertex of T , then T is a star and by Lemmas 2.1 and 2.2, $\eta(G) = \eta(G - T) + \nu(T) - 2 = \eta(G - T) + \eta(T)$. Otherwise, let $w \in T$ ($w \neq u$) be a quasi-pendent vertex adjacent to the pendent vertex $w' \in T$. Let the components of $T - w - w'$ be T_1, T_2, \dots, T_s ($s \geq 1$), where T_1 contains the vertex u . We claim that u is still perfectly matched in T_1 . Consider a maximal matching M of T , where M contains a pendent edge e_w joining w and w' . Then $M = M_1 \cup M_2 \cup \cdots \cup M_s \cup e_w$, where $M_i = M \cap E(T_i)$ is still a maximal matching of T_i for $i = 1, 2, \dots, s$. If u is not perfectly matched in T_1 , then T_1 has a maximal matching such that u is not matched by this matching, and in turn T has a maximum matching such that u is not matched by this matching, a contradiction to the

definition of u . Note that $e(T_1) < m$, and then by Lemmas 2.1 and 2.2 and by induction,

$$\begin{aligned}\eta(G) &= \eta(G - w - w') = \sum_{i=2}^s \eta(T_i) + \eta(G - \sum_{i=2}^s T_i - w - w') \quad (\text{by Lemmas 2.1, 2.2}) \\ &= \sum_{i=2}^s \eta(T_i) + \eta((G - \sum_{i=2}^s T_i - w - w') - T_1) + \eta(T_1) \quad (\text{by induction}) \\ &= \sum_{i=1}^s \eta(T_i) + \eta(G - T) = \eta(T) + \eta(G - T) \quad (\text{by Lemma 2.1}).\end{aligned}$$

(ii) Using induction principle on $e(T)$. Since u is mismatched in T , $e(T) \neq 1$. And without loss of generality, let $e(T) \geq 2$. If $e(T) = 2$, $T = P_3 = uvw$, by Lemma 2.1, $\eta(G) = 0 + \eta(G - v - w) = \eta(T - u) + \eta(G - (T - u))$. Suppose the result holds for all trees T with $e(T) < m$. Now we consider the case of $e(T) = m$. If T is a star, u must be a pendent vertex for it is mismatched in T , and by Lemmas 2.1 and 2.2, $\eta(G) = \eta(G - (T - u)) + \nu(T) - 3 = \eta(G - (T - u)) + \eta(T - u)$. Otherwise, let $w \in T$ ($w \neq u$) be a quasi-pendent vertex adjacent to the pendent vertex $w' \in T$. Let the components of $T - w - w'$ be T_1, T_2, \dots, T_s ($s \geq 1$), where T_1 contains the vertex u . We claim that u is still mismatched in T_1 . Consider a maximal matching M of T , where M contains a pendent edge e_w joining w and w' , and u is mismatched in M . Then $M = M_1 \cup M_2 \cup \dots \cup M_s \cup e_w$, where $M_i = M \cap E(T_i)$ is still a maximal matching of T_i for $i = 1, 2, \dots, s$. If u is perfectly matched in T_1 , then T_1 has a maximal matching such that u is not matched by this matching. Note that $e(T_1) < m$, and then by Lemmas 2.1 and 2.2 and by induction,

$$\begin{aligned}\eta(G) &= \eta(G - w - w') = \sum_{i=2}^s \eta(T_i) + \eta(G - \sum_{i=2}^s T_i - w - w') \quad (\text{by Lemmas 2.1, 2.2}) \\ &= \sum_{i=2}^s \eta(T_i) + \eta((G - \sum_{i=2}^s T_i - w - w') - (T_1 - u)) + \eta(T_1 - u) \quad (\text{by induction}) \\ &= \sum_{i=2}^s \eta(T_i) + \eta(T_1 - u) + \eta(G - (T - u)) \\ &= \eta(T - u) + \eta(G - (T - u)) \quad (\text{by Lemma 2.1}). \quad \square\end{aligned}$$

Corollary 2.6 *Let u be a mismatched vertex of a tree T . Then $\eta(T - u) = \eta(T) - 1$.*

We call U an elementary unicyclic graph if it satisfies

(a) U is the cycle C_n where $n \not\equiv 0 \pmod{4}$; or

(b) U is obtained from C_n and tK_1 by the rule: First select t vertices from C_n 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 chosen in C_n to an isolated vertex.

We denote by $NS(\mu)$ and \mathcal{U}_0 respectively the set of nonsingular unicyclic graph on n vertices, and the set of unicyclic graph which satisfies the condition: $G \in \mathcal{U}_0$ is an elementary unicyclic graph or a unicyclic graph obtained by joining a vertex of PM-trees with an arbitrary vertex of an elementary unicyclic graph.

Theorem 2.7 ([6, 7]) *Let G be a unicyclic graph. Then $\eta(G) = 0$ if and only if $G \in \mathcal{U}_0$.*

3. Unicyclic graphs with nullity one

A unicyclic graph G is called a second-elementary unicyclic graph if U is obtained from an even cycle by attaching a pendent edge (see Figure 3 (i)), or is obtained from an odd cycle by attaching one pendent edge at two distinct vertices respectively (see Figure 3 (ii)), or is obtained from a cycle C_n by attaching one pendent edge at t ($t \equiv n - 1 \pmod{2}, t > 2$) distinct vertices such that there are an odd number of vertices on the cycle lying between exactly one pair of consecutive vertices of these t vertices, and there are an even number (possibly zero) of vertices on the cycle lying between any other pair of consecutive vertices (see Figure 3 (iii)). Let G be a second-elementary unicyclic graph, deleting the t pendent vertices together with their neighbors one by one. We get a set of separate paths and there is but one path with odd cardinality. By Lemmas 2.1 and 2.2, $\eta(G) = 1$.

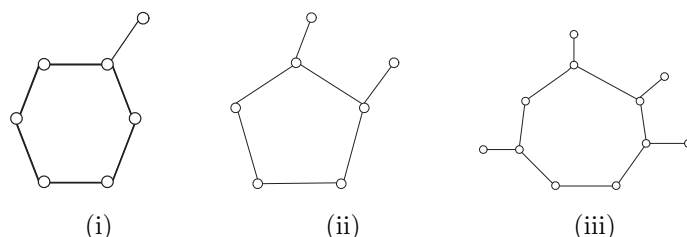


Figure 3 Illustration of the second-elementary unicyclic graphs

Denote by \mathcal{U}_1 the set of unicyclic graphs which satisfy one of the following conditions:

- (i) G is a second-elementary unicyclic graph;
- (ii) G is obtained by joining one vertex of each of several PM-trees to an arbitrary vertex of a second-elementary unicyclic graph (see Figure 4(i));
- (iii) G is obtained from the graph as in (ii) by the rule: First, join a mismatched vertex of a tree with nullity one to an arbitrary quasi-pendent vertex of an elementary unicyclic graph. Then join one vertex of each of several PM-trees to an arbitrary vertex of the elementary unicyclic graph (see Figure 4(ii));
- (iv) G is a unicyclic graph obtained by the rule: First, join a perfectly matched vertex of a tree with nullity one with an arbitrary vertex of an elementary unicyclic graph. Then join one vertex of each of several PM-trees to an arbitrary vertex of the elementary unicyclic graph (see Figure 4(iii)).

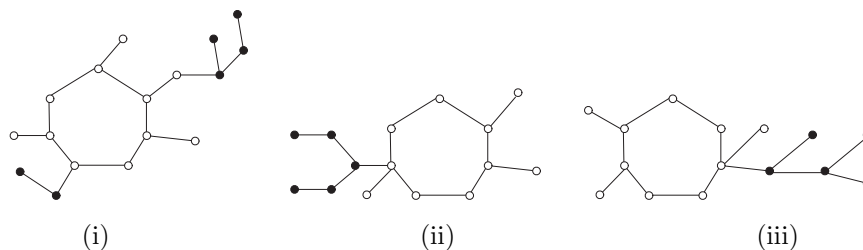


Figure 4 Examples of the graphs in \mathcal{U}_1

Let G be a unicyclic graph with $\eta(G) = 1$. By Lemma 2.3, G is not a cycle. Let C_n be the cycle of G and $V(C_n) = \{v_i : i = 1, 2, \dots, n\}$, and $G - E(C_n) = T_1 \cup T_2 \cup \dots \cup T_n$, where T_1, T_2, \dots, T_n are the set of trees in $G - E(C_n)$ containing vertices v_1, v_2, \dots, v_n , respectively.

Assertion 3.1 *If for some i , v_i is a mismatched vertex of T_i . By Lemma 2.5 (ii), $\eta(G) = \eta(G - (T_i - v_i)) + \eta(T_i - v_i) = 1$, thus $\eta(T_i - v_i) \leq 1$.*

Assertion 3.2 *If for some i , v_i is a perfectly matched vertex of T_i . By Lemma 2.5 (i), $\eta(G) = \eta(G - T_i) + \eta(T_i) = 1$, thus $\eta(T_i) \leq 1$.*

For simplicity, we introduce the following notations:

$$\begin{aligned} T_{m0} &= \{T \in T_i \mid v_i \text{ is a mismatched vertex of } T_i \text{ and } \eta(T_i - v_i) = 0\}; \\ T_{m1} &= \{T \in T_i \mid v_i \text{ is a mismatched vertex of } T_i \text{ and } \eta(T_i - v_i) = 1\}; \\ T_{p0} &= \{T \in T_i \mid v_i \text{ is a perfectly matched vertex of } T_i \text{ and } \eta(T_i) = 0\}; \\ T_{p1} &= \{T \in T_i \mid v_i \text{ is a perfectly matched vertex of } T_i \text{ and } \eta(T_i) = 1\}. \end{aligned}$$

Assertion 3.3 $T_{m1} \cup T_{p0} \cup T_{p1} \neq \emptyset$.

Proof If for all i ($1 \leq i \leq n$), v_i is a mismatched vertex of T_i and $\eta(T_i - v_i) = 0$, then applying Lemma 2.5 (ii) repeatedly, $\eta(G) = \eta(C_n) + \sum_{i=1}^n \eta(T_i - v_i) = 1$. Thus $\eta(C_n) = 1$, which is impossible. \square

Assertion 3.4 *Let U be an elementary unicyclic graph and u be one of its pendent vertices, $N_U(u) = u_0$. Then $\eta(U + u_0v) = 1$, where v is an isolated vertex.*

Proof By Lemmas 2.1 and 2.2, $\eta(U + u_0v) = \eta(U - u_0 - u) + \eta(K_1) = \eta(U) + \eta(K_1) = 1$. \square

Theorem 3.5 *Let G be a unicyclic graph. Then $\eta(G) = 1$ if and only if $G \in \mathcal{U}_1$.*

Proof (\Rightarrow) We carry out the proof in three cases.

Case 1 If $T_{m1} \neq \emptyset$, then for some i , v_i is a mismatched vertex of T_i , $\eta(T_i - v_i) = 1$. There is one but only one component of $T_i - v_i$ with nullity one (others zero). Let it be T_0 and $v_0 \in T_0$ join with v_i . Since v_i is mismatched in T_i , v_0 must be perfectly matched in T_0 (or else, $\eta(T_i - v_i - v_0) = 0$ and $T_i - v_i - v_0$ is a PM-acyclic graph, we add edge v_0v_i to a perfect matching of $T_i - v_i - v_0$, then we would get that T_i is a PM-tree, contradiction). And in this case $G - (T_i - v_i)$ is a unicyclic graph with nullity zero. By Theorem 2.7, G satisfies condition (iv).

Case 2 If $T_{p1} \neq \emptyset$, then for some i , v_i is a perfectly matched vertex of T_i and $\eta(T_i) = 1$. Let $M(T_i)$ be one of its maximal matchings, $uv_i \in M(T_i)$. Then $\eta(T - u - v_i) = 1$ and there is one but only one component of $T_i - u - v_i$ with nullity one (others zero). Let it be T_0 and $v_0 \in T_0$ join with v_i or u . If v_0 is adjacent to u , v_0 must be a perfectly matched vertex of T_0 (or else replace uv_i by uv_0 in $M(T_i)$, we get another maximal matching of T_i and v_i is mismatched, contradiction). But no matter in what cases, by Lemma 2.5 (i), $\eta(G - T_0) = \eta(G) - \eta(T_0) = 0$, $G - T_0$ is a unicyclic graph with nullity zero. By Theorem 2.7, G satisfies condition (iii) or (iv).

Case 3 If $T_{m1} = \emptyset$, $T_{p1} = \emptyset$, by Assertion 3.3, $T_{p0} \neq \emptyset$. Then G must satisfy condition (i) or (ii). By applying Lemma 2.5 repeatedly, $\eta(G) = \eta(C_n - \bigcup_{T_i \in T_{p0}} v_i) + \sum_{T_i \in T_{m0}} \eta(T_i - v_i) + \sum_{T_i \in T_{p0}} \eta(T_i) = \eta(C_n - \bigcup_{T_i \in T_{p0}} v_i) = 1$, and $C_n - \bigcup_{T_i \in T_{p0}} v_i$ is composed of some paths. Then there is but one odd-path which implies that:

- (a) C_n is an even cycle, when $|T_{p0}| = 1$;
- (b) C_n is an odd cycle, when $|T_{p0}| = 2$;
- (c) There is but one pair of consecutive vertices of $\{v_i \in T_i \mid T_i \in T_{p0}\} \subseteq C_n$ with an odd number of vertices in C_n between them, when $|T_{p0}| > 2$.

For each $T_i \in T_{p0}$, v_i is a perfectly matched vertex of T_i and T_i is a PM-tree. Let $M(T_i)$ be one of its perfect matchings, and $uv_i \in M(T_i)$. By Theorem 2.4, each component of $T - u - v_i$ is a PM-tree, and they are joined with u or v_i by an edge.

For each $T_i \in T_{m0}$, v_i is a *mismatched* vertex of T_i (here $T_i \neq K_1$). Since $\eta(T_i - v_i) = 0$, by Lemma 2.2 and Theorem 2.4, the nullity of each component of $T_i - v_i$ is zero and they are all PM-trees joining with v_i by an edge.

Now we have G is a second-elementary unicyclic graph (when $T_{m0} = \emptyset$ and for all $T_i \in T_{p0}$, $T_i = P_2$), or G is a unicyclic graph obtained by joining a vertex of PM-trees with an arbitrary vertex of a second-elementary unicyclic graph, repeatedly.

Summarizing the above, we complete the proof of the necessity.

(\Leftarrow) We verify each possible cases.

If G is a unicyclic graph which satisfies condition (i), $\eta(G) = 1$.

If G is a unicyclic graph which satisfies condition (ii), then by applying Lemma 2.5 (i) repeatedly, we have $\eta(G) = \eta(S) = 1$, where S is a second-elementary unicyclic graph.

If G is a unicyclic graph satisfying condition (iii). Let U be an elementary unicyclic graph and u be one of its pendent vertices, $N_U(u) = u_0$. Let T_1 be a tree with nullity one, \mathcal{T}_p be a set of disjoint PM-trees, and v be a mismatched vertex of T_1 . G is obtained by joining v with u_0 , and joining a vertex of PM-trees $\in \mathcal{T}_p$ with an arbitrary vertex of U , repeatedly. Then by Corollary 2.6, $\eta(T_1 - v) = 0$. Using Lemma 2.5 repeatedly, we have

$$\eta(G) = \eta(T_1 - v) + \sum_{T \in \mathcal{T}_p} \eta(T) + \eta(U + u_0v) = \eta(U + u_0v).$$

By Assertion 3.4, $\eta(G) = 1$.

If G is a unicyclic graph satisfying condition (iv), with the similar discussion as above, by applying Lemma 2.5 repeatedly, we have

$$\eta(G) = \eta(T_1) + \sum_{T \in \mathcal{T}_p} \eta(T) + \eta(U) = \eta(T_1) = 1.$$

The proof of sufficiency is completed. \square

In paper [8], the author determined another necessary and sufficient condition for a graph G to be singular for acyclic and unicyclic graphs.

A pair V_1, V_2 of subsets of $V(G)$ is said to satisfy the property (N) if V_1 and V_2 are nonempty and disjoint and $\{N(v) \mid v \in V_1\} = \{N(v) \mid v \in V_2\}$.

Theorem 3.6 (see [8]) *A unicyclic graph G is singular if and only if there is a pair of subsets V_1 and V_2 of $V(G)$ satisfying the property (N).*

Using the same method, we also have

Theorem 3.7 *Let G be a unicyclic graph. Then $\eta(G) = 1$ if and only if there is a pair of subsets V_1 and V_2 of $V(G)$ satisfying the property (N), and there exists a vertex $u \in V(G)$ such that $G - u$ contains no such pair of subsets.*

Example 3.8 Consider the graphs in Figure 5.

(a) $\eta(G) > 1$, there is a pair of subsets V_1 and V_2 of $V(G)$ satisfying the property (N), and for each vertex $u \in V(G)$, $G - u$ still contains such pair of subsets;

(b) $\eta(G) = 1$, there is a pair of subsets V_1 and V_2 of $V(G)$ satisfying the property (N), and there exists a vertex $u \in V(G)$, such that $G - u$ contains no such pair of subsets;

(c) $\eta(G) = 0$, there exist no pair of subsets V_1 and V_2 of $V(G)$ satisfying the property (N).

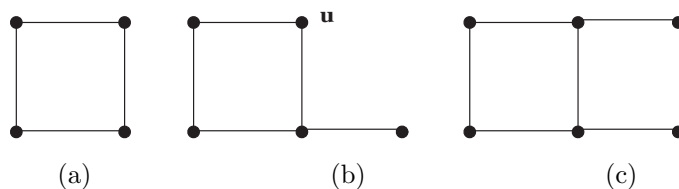


Figure 5 Examples of Theorems 3.6 and 3.7

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