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Energy of a set of vertices in a Graph

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Abstract

Given a finite graph $G=(V,E)$, and any proper subset D of the vertex set $V := V(G)$ of G, we associate a nonnegative integral matrix $A_D(G)=(a_{ij})$ of order $|D|\times|D|$ with D so that the i^{th} diagonal entry in the matrix counts precisely the number of edges that join the i^{th} vertex of D with vertices in $V-D$ so that these *partial degrees* of the vertices in D are precisely the *eigenvalues* of $A_D(G)$ whence their sum may be conceived as the energy $\varepsilon_D(G)$ of the given set D. Invoking the underlying notion of *incidence matrix* of D, we introduce in this paper the notion of *robust domination energy* (or, *rd-energy*) and *shear domination energy* (or, *sd-energy*) of G as the maximum (minimum, respectively) energy of a minimal dominating set in G. We raise several interesting open problems and connections of these notions with other well known ones in graph theory.

Keywords: Robust domination energy, shear domination energy.

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1. Preamble

The strength of a social group D in a society depends not only on how tightly its members are bound (or, 'knit') amongst themselves but also on how well connected they are by relations to individuals outside the group. While the in-group relations in D account for the amount of cohesion (or, 'solidarity') amongst the members of the group, the out-group relations of D indicate how well the group is 'embedded' in the larger social system; the latter accounts for the effect of the 'environment' or the 'external system' in the casuality of the very in-group interactions and relations (Cartwright and Harary [4]; Everett and Nieminen [3]; Seidman [8]-[11]). While in-group cohesion appears to be a well-studied socio-psychological phenomenon, the study of a group's connections to its external system seems to have been relatively limited. A pertinent remark in this context is by Reis et al. [7]:

The individualistic perspective that seeks the cause of behavior within the properties of the single individual must be augmented, and in some cases replaced, by the methods for seeking the cause of behavior within the interconnections of individuals and their relationship as well as the interconnections between those relationships and the larger systems within which they are embedded.

If we are allowed to extrapolate this view in the social context, it appears quite plausible to us to replace the term 'individual' in the above view of Reis et al. [7] by the term 'social group' towards extending its validity to have a systematic approach to study the dynamics of *group behavior*. These considerations have motivated us to think of a network approach and introduce application of the well known notion of domination in graphs to define what we shall refer to as *energy* of a dominating set (or, 'domset' in short) in a given graph. Since interaction between members of a dyad generally occurs on several issues or attributes of common concern between them, often simultaneously, each of the multiple edges standing for one of the issues/attributes of their common concern, multigraphs are useful in such cases (*e.g.,* see Peay [5],[6]; Acharya and Acharya,[1]; Acharya [2]).

2. Introduction

In this paper, unless mentioned otherwise, the terminology and notions in graph theory will be as in West [12] and by a graph we shall mean a finite simple graph without loops and multiple edges.

Given a graph $G = (V, E)$ of order n and a nonempty proper subset $D \subset V$, say $D = \{u_1, u_2, \ldots, u_t\}$, we define the *boundary matrix* $B_D(G) = (b_{ij})_{t\times(n-t)}$ of D by letting b_{ij} to be the number of edges that join the i^{th} vertex u_i of D to the j^{th} vertex v_j of $V - D$. Clearly then, the i^{th} row sum of $B_D(G)$ yields the number of edges that join u_i to the vertices of $V - D$, so called *partial degree* $d_D(u_i)$ of u_i with respect to the given set D, and the sum $\sum_{i=1}^{t} d_D(u_i)$ gives precisely the number $m(D, V - D)$ of *boundary edges* of D, viz., the edges that join the vertices of D with those of its *complement* $\overline{D} = V - D$.

Given a graph $G = (V, E)$, a subset $D \subseteq V$ is called a *dominating set* (or, simply a *domset*) of G if every vertex in G is either in D or is adjacent to a vertex in D. The set of all domsets in G is denoted by $\mathcal{D}(G)$. A domset is *minimal* if no proper subset of it is a domset of G and *minimum* if it has the least number $\gamma(G)$ of vertices amongst all the domsets in G; accordingly, the set of all minimal (minimum, respectively) domsets in G is denoted $\mathcal{D}^m(G)(\mathcal{D}^0(G))$.

Proposition 2.1. *If D is a proper domset of a graph $G = (V, E)$ then every column of $B_D(G)$ has a nonzero entry. Further, if $D \in \mathcal{D}^m(G)$ then every row of $B_D(G)$ contains a nonzero entry too.*

Proof. The first statement follows by the very definition of domset in G. The second statement in the proposition follows from the well known fact that if D is a minimal dominating set of G then $V - D$ is a domset too. (e.g., see Haynes et al, 1997). □

Now, consider the matrix product

$$A_D(G) = B_D(G) \cdot B_D(G)^T = (a_{ij})_{t\times t}$$

where " · " means usual matrix multiplication and $B_D(G)^T$ denotes the *transpose* of the boundary matrix $B_D(G)$. Then the *energy* of D, denoted $\varepsilon_G(D)$, is defined as the sum $\sum_{i=1}^{|D|} |\mu_i|$, where μ_i are the eigenvalues of $A_D(G)$ and $|\mu_i|$ is the usual modulus (called the *magnitude*) of the number μ_i.

Note that D is a proper subset of $V(G)$ by choice in this definition of $\varepsilon_G(D)$. The definition of energy ε_G of G, defined similarly as the sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$ of G, which originally comes from molecular chemistry, corresponds to taking $D = V(G)$ in the above definition of $\varepsilon_G(D)$. This mathematical extension of the meaning of $\varepsilon_G(D)$ with that of ε_G when $D = V(G)$ needs appropriate understanding in terms of molecular chemistry.

The *robust domination energy* (*rd-energy*, in short) of the graph G, denoted $\varepsilon_{rd}(G)$, is defined as the quantity $max\{\varepsilon_G(D) : D \in \mathcal{D}^m(G)\}$, and the *shear domination energy* (*sd-energy*, in short) of the graph G, denoted $\varepsilon_{sd}(G)$, is defined as the quantity $min\{\varepsilon_G(D) : D \in \mathcal{D}^m(G)\}$.

At this stage, it is important to observe that $\varepsilon_{sd}(G)$ may be attained by a minimal domset which is not a minimum domset; for example, take the graph G denoted $2MK_6$, which is obtained as follows: Take the complete graph K_6 on the vertex set $V = \{1', x, 2', 3', y, 4'\}$, take four new vertices $1, 2, 3, 4$ and join them to the vertices in V by the new edges $11', 22', 33', 44', 1x, 2x, 3y, 4y$. This graph has $D_1 = \{x, y\}$ as the unique minimum domset and for which $\varepsilon_G(D_1) = 12$, whereas $D = \{1, 2, 3, 4\}$ is a minimal dominating set for which $\varepsilon_G(D) = 8$, so that

$$\varepsilon_{sd}(G) \leq \varepsilon_G(D) = 8 < 12 = \varepsilon_G(D_1).$$

Hence for any integer $n \geq 2$, if $\mathcal{G}_n(d)$ denotes the set of all graphs of order n with domination number d, then we let $\varepsilon^0_{rd}(n,d) = min\{\varepsilon_{rd}(G) : G \in \mathcal{G}_n(d)\}$, $\varepsilon^1_{rd}(n,d) = max\{\varepsilon_{rd}(G) : G \in \mathcal{G}_n(d)\}$, $\varepsilon^0_{sd}(n,d) = min\{\varepsilon_{sd}(G) : G \in \mathcal{G}_n(d)\}$ and $\varepsilon^1_{sd}(n,d) = max\{\varepsilon_{sd}(G) : G \in \mathcal{G}_n(d)\}$. Also, define $\varepsilon^{1*}_{rd}(n,d) = max\{\varepsilon_D(G) : G \in \mathcal{G}_n(d), D \in \mathcal{D}^0(G)\}$. Similarly, $\varepsilon^{0*}_{rd}(n,d), \varepsilon^{1*}_{sd}(n,d)$ and $\varepsilon^{0*}_{sd}(n,d)$ are defined. It will be of fundamental importance to find tight bounds for, if not exact values of, these invariants.

3. Results

The following lemma is basic and gives us an easy method to calculate the domination energies.

Lemma 3.1. *Let D be any minimal domset of any graph G of order $n \geq 2$ and let $D = \{u_1, u_2, \ldots, u_t\}$. Then*

(i) *$A_D(G)$ is a nonnegative semidefinite symmetric matrix of order t; and*

(ii) *$\varepsilon_G(D) = m(D, V-D)$.*

Proof. (i) $A_D(G)$ is a symmetric matrix, as

$$A_D(G)^T = (B_D(G)^T)^T \cdot B_D(G)^T = A_D(G).$$

Further, $A_D(G)$ is a nonnegative semidefinite quadratic form and hence the eigenvalues of $A_D(G)$ are all nonnegative. (Let X be a real row vector of length t; then

$$X \cdot A_D(G) \cdot X^T = X \cdot B_D(G) \cdot B_D(G)^T \cdot X^T = Y \cdot Y^T = \sum_{i=1}^{n-t} y_i^2 \geq 0$$

where $Y = X \cdot B_D(G)$). Note, that $X \cdot B_D(G)$ is a row vector of length $(n-t)$ and $B_D(G)^T \cdot X^T$ is a column vector of length $(n-t)$. Hence, all the eigenvalues of $A_D(G)$ are nonnegative.

(ii) Further, the i^{th} diagonal entry of the matrix $A_D(G)$ counts precisely the number of edges that join the i^{th} vertex of D with vertices of $V-D$ whence their sum is the energy $\varepsilon_D(G)$ of the given domset D of G. Hence,

$$\varepsilon_D(G) = \sum_{i=1}^{|D|} |\mu_i| = \sum_{i=1}^{|D|} \mu_i$$

which, by (i), is equal to the trace of the matrix $A_D(G)$. Therefore, $\varepsilon_G(D)$ is equal to the sum of the partial degrees of the vertices of D in the spanning bipartite graph $G(D, V-D)$ consisting of the boundary edges of D; in other words $\varepsilon_G(D) = m(D, V-D)$. □

Problem 3.2. *Let $\mathcal{P}$ be an invariant property of graphs; for example:*

- *$\mathcal{P}$ is a tree,*
- *$\mathcal{P}$ is a planar graph,*
- *$\mathcal{P}_k$: chromatic number $\leq k$,*

Find the values of $\varepsilon^0_{rd}(\mathcal{P}, n), \varepsilon^1_{rd}(\mathcal{P}, n), \varepsilon^0_{sd}(\mathcal{P}, n)$ and $\varepsilon^1_{sd}(\mathcal{P}, n)$, as well as the $\varepsilon^{1*}_{rd}(\mathcal{P}, n), \varepsilon^{0*}_{rd}(\mathcal{P}, n), \varepsilon^{1*}_{sd}(\mathcal{P}, n)$ and $\varepsilon^{0*}_{sd}(\mathcal{P}, n)$ restricted over all simple graphs of order n with the property $\mathcal{P}$.

Problem 3.3. *Find the values of $\varepsilon^0_{rd}(\mathcal{P}, n, d), \varepsilon^1_{rd}(\mathcal{P}, n, d), \varepsilon^0_{sd}(\mathcal{P}, n, d)$ and $\varepsilon^1_{sd}(\mathcal{P}, n, d)$, as well as $\varepsilon^{1*}_{rd}(\mathcal{P}, n, d), \varepsilon^{0*}_{rd}(\mathcal{P}, n, d), \varepsilon^{1*}_{sd}(\mathcal{P}, n, d)$ and $\varepsilon^{0*}_{sd}(\mathcal{P}, n, d)$ restricted over graphs with $\gamma(G) = d$, of order n with the property $\mathcal{P}$. Characterise all the extremal graphs in each case for each property $\mathcal{P}$.*

Lemma 3.4. *For any simple graph $G = (V, E)$ having size q, $\varepsilon_{rd}(G) = q$ if and only if G is bipartite.*

Proof. Suppose $\varepsilon_{sd}(G) = q$. Then there exists $D \in \mathcal{D}^m(G)$ such that $\varepsilon_G(D) = m(D, V - D) = \varepsilon_{rd}(G) = q$. This implies that both D and $V - D$ are independent whence it is easy to see that $G = G(D, V - D)$ is bipartite.

Conversely, if $G = G(V_1, V_2)$ is a bipartite graph with $|V_1| \leq |V_2|$, then $m(V_1, V_2) = q \leq \varepsilon_{rd}(G)$. Since $\varepsilon_{rd}(G) \leq q$ obviously, the result follows. □

Theorem 3.5. *The minimum energy of a minimal domset in a connected simple graph G of order $n \geq 2$ is $\lceil \frac{n}{2} \rceil$ and the bound is sharp.*

Proof. Let G be a graph of order $n \geq 2$ and D be a minimal domset of G with cardinality d. Then every vertex of $V - D$ is adjacent to a vertex in D and therefore, the number of edges between $V - D$ and D is at least $n - d$. Therefore, the energy of D is at least $n - d$.

On the other hand if x is the number of vertices in D each of which has a private neighbor in $V - D$, then each of the remaining $d - x$ vertices is an isolate in D, and as G is connected each of these $d - x$ vertices is adjacent to a vertex in $V - D$ and therefore, there are at least d edges from D to $V - D$. Thus, the energy of D is at least d. Therefore, the energy of D is at least the maximum of d and $n - d$, and hence the energy of G is at least as much as asserted.

To prove the bound is the best possible, we consider the following two cases:

Case 1. n is even and $n = 2s$.

Let G be the graph consisting of a connected graph H on s vertices and exactly one pendant new edge attached at each of its vertices of H. This graph has the minimum (shear) domination energy equal to s.

Case 2. $n = 2s + 1$.

Then we take the above graph on $2s$ vertices and add a new edge at one of the vertices of H above to get a graph whose minimum domination energy is $s + 1$. □

Theorem 3.6. *The maximum energy of a simple graph G of order n is $\lfloor \frac{n^2}{4} \rfloor$ and the bound is sharp.*

Proof. Let D be a minimal domset of cardinality d. Then the energy of G with respect to this D is at most $d(n-d)$ which is at most the number given in the statement of this theorem as $d+(n-d) = n$ is a constant. This bound is attained by the complete bipartite graph on n vertices where both parts of the bipartition have almost equal cardinality. This is true as both parts of the bipartition are minimal domsets or by the fact that in a bipartite graph with m edges, the maximum domination energy is m. This completes the proof. □

Theorem 3.7. *Let n and d be positive integers with $d \geq 3$ and $n \geq d(d-1)+1$. Then $\varepsilon^{1*}_{rd}(n, d) = d(n - 2d + 2) - 1$.*

Proof. Let $f(n, d) = d(n - 2d + 2) - 1$ and $g(n, d) = d(n - d)$, where $n \geq d(d-1)+1$, with fixed integer $d \geq 3$. Let $\mathcal{G}^*(n, d) = \{G^* = G(n, d)\}$ be the set of all graphs with vertex set $A^* \cup B^* \cup C^*$, where $A^* = \{u^*_1, u^*_2, \ldots, u^*_d\}, B^* = \{v^*_1, v^*_2, \ldots, v^*_{d-1}\}$ and $C^* = \{x^*_1, x^*_2, \ldots, x^*_t\}$, where $t = n-2d+1$; and edges are $(u^*_i, v^*_i), 1 \leq i \leq d-1$, $(u^*_j, x^*_k), 1 \leq j \leq d$ and $1 \leq k \leq t$, and optional edges are $(u^*_i, u^*_l), 1 \leq i < l \leq d-1$ and $(x^*_j, x^*_r), 1 \leq j < r \leq t$. It is easy to see that domination number of $G^* \in \mathcal{G}^*(n, d)$ is d with A^* as minimum dominating set, and $\varepsilon_D(G^*) = d(n-2d+1)+(d-1) = d(n-2d+2)-1 = f(n, d)$. Thus,

$$f(n, d) \leq \varepsilon^{1*}_{rd}(n, d) \leq d(n - d) = g(n, d). \tag{1}$$

Let G be a graph of order n with $\gamma(G) = d$, and $D = \{u_1, u_2, \ldots, u_d\}$ be a minimum dominating set and $D = \{u_1, u_2, \ldots, u_d\}$ with $\varepsilon_D(G) > f(n, d)$, if possible. Then the number of edges in $\overline{G}$, the complement of G, between D and $V(G) - D$ is at most

$$g(n, d) - f(n, d) - 1 = d(d - 2). \tag{2}$$

As $n \geq d(d-1)+1$, $|V - D| \geq d(d-2)+1$, and hence by (2) there exists a vertex v^* in $V - D$ such that v^* is adjacent to all the vertices in D. Fix such a vertex v^*.

Let now $\{v_1, v_2, \ldots, v_t\}$ be the set of all vertices in $V - D$, each of which is nonadjacent to a fixed vertex u_1 (say) of D. If $t \leq d-3$, then $\{u_1, v_1, v_2, \ldots, v_t, v^*\}$ is a domset of G of cardinality at most $d-1$. As $\gamma(G) = d$, it follows that $t \geq d-2$. Thus, each u_i of D is nonadjacent to at least $d-2$ vertices of $V - D$.

By (2), it follows that each u_i is nonadjacent to exactly $d-2$ vertices of $V - D$. (3)

Without loss of generality, let $v_1, v_2, \ldots, v_{d-2}$ be the vertices nonadjacent in G to the vertex u_1 of D. As D is a domset of G, each of the vertices $v_i, 1 \leq i \leq d-2$, is adjacent to some vertex u_i of D. If now $v_i, v_l, 1 \leq i < l \leq d-2$ are adjacent to the same u_j in D, then $\{v^*, u_1, u_j, v_1, \ldots, v_{d-2}\} - \{v_i, v_l\}$ is a domset of G of cardinality $d-1$, which is a contradiction.

Thus, in G each v_i is adjacent to exactly one vertex in D and distinct $v_i, 1 \leq i \leq d-2$, are adjacent in G to distinct vertices in D. Without loss of generality, let v_i be adjacent to $u_{i+1}, 1 \leq i \leq d-2$, in G.

From above it is clear that each $u_i, 2 \leq i \leq d-1$, is nonadjacent in G to exactly one vertex of $V-D$ outside $\{v_1, v_2, \ldots, v_{d-2}\} = B$ (say). Then $D^* = \{u_2, u_3, \ldots, u_{d-1}, v^*\}$ is a domset of G of cardinality $d-1$, unless $u_2, u_3, \ldots, u_{d-1}$ are all nonadjacent to the same vertex v^{**} of $V-D$, not in B. Notice that u_1 is adjacent in G to v^{**}, as v^{**} is not in B.

If $(u_d, v_i), 1 \leq i \leq d-2$ for some i is an edge of G, then $A \cup \{v_i\} - \{u_{i+1}, u_d\}$ is a domset of G of cardinality $d-1$. Similarly, if (u_d, v^{**}) is an edge of G, then $A \cup \{v^{**}\} - \{u_1, u_d\}$ is a domset of G of cardinality $d-1$. If (u_i, u_d) is an edge of G for some $i, 1 \leq i \leq d-1$, then $\{u_1, u_2, \ldots, u_{d-1}\}$ is a domset of G of cardinality $d-1$. Thus, u_d is not adjacent to any vertex of $B \cup \{v^{**}\}$, contradicting (3). This completes the proof of the theorem. □

Problem 3.8. *Find the values of* $\varepsilon^0_{rd}(n,d), \varepsilon^1_{rd}(n,d), \varepsilon^0_{sd}(n,d), \varepsilon^1_{sd}(n,d)$ *and also* $\varepsilon^{1*}_{rd}(n,d), \varepsilon^{0*}_{rd}(n,d), \varepsilon^{1*}_{sd}(n,d), \varepsilon^{0*}_{sd}(n,d)$, *for all admissible values of* n, *and also characterise the extremal graphs in each case.*

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