ENERGY, DISTANCE ENERGY OF CONNECTED GRAPHS AND SKEW ENERGY OF CONNECTED DIGRAPHS WITH RESPECT TO ITS SPANNING TREES AND ITS CHORDS

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ABSTRACT: The energy of a graph G is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. The distance energy of a graph G is defined as the sum of the absolute values of the D-eigen values of its distance matrix. The skew energy of a graph G is defined as the sum of the absolute values of the eigenvalues of its skew adjacency matrix. Jane Day and Wasin So, [2007] have discussed about the changes in the energy of the graph due to the deletion of edges. In this paper the changes of energy, distance energy of connected graphs and the skew energy of connected digraphs are studied with respect to its spanning trees and its chords.

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KEYWORDS: Connected graphs, Connected digraphs, Spanning trees, Graph energy, Distance energy, Skew energy.

1. INTRODUCTION

Graphs can be used to represent any physical situation involving discrete objects among them. In general, graph theory has its impact on each and every branch of science. In Mathematics and Computer Science, connectivity is one of the basic concepts of graph theory. It is closely related to the theory of network flow problems. The connectivity of a graph is an important measure of its robustness as a network. One of the important facts about connectivity in graphs is Menger's theorem, which characterizes the connectivity and edge connectivity of a graph in terms of the number of independent paths between vertices. Connected graphs are useful for characterization and identification of chemical compounds. A connected graph is used to represent a chemical compound with vertices as the atoms and the edges for representing the bonds between the atoms. Cayley showed that every group of order n can be represented by a strongly connected digraph of n vertices, in which each vertex corresponds to a group element and edges carry the label of a generator of the group. Cayley used edges of different colors to show different generators. We can say that a graph of a cyclic group of order n is a directed circuit of n vertices in which every vertex has the same label. Also the digraph of a group uniquely defines the group by specifying how every product of elements corresponds to a directed

edge sequence. This digraph known as the Cayley diagram is useful in visualizing and studying abstract groups.

The concept of energy of a graph arose in chemistry, where certain numerical quantities, such as the heat formation of a hydrocarbon are related to the so-called total π-electron energy that can be calculated from the energy of the corresponding molecular graph. The energy of a simple graph G was first defined by Ivan Gutman [12] in 1978 as the sum of the absolute values of the eigenvalues of its adjacency matrix. The molecular graph is the representation of molecular structure of a hydrocarbon, whose vertices are the position of carbon atoms and two vertices are adjacent, if there is a bond connecting them. In chemistry, molecular orbital theory (MO) is a method for determining molecular structure in which electrons are not assigned to individual bonds between atoms, but are treated as moving under the influence of the nuclei in the whole molecule. In this theory, each molecule has a set of molecular orbitals in which it is assumed that the molecular orbital wave function Ψ_f may be written as a simple weighted sum of the n constituent atomic orbitals χ_i according to the following equation $\Psi_j = \sum_{i=1}^{n} c_{ij} \chi_i$, where the co-efficients c_{ij} may be determined numerically using Schrodinger equation and application of the variational principle.

The Huckel method or Huckel molecular orbital method (HMO) proposed by Erich Huckel in 1930, is a very simple linear combination of atomic orbitals-molecular orbitals (LCAO-MO) method for the determination of energies of molecular orbitals of pi electrons in conjugated hydrocarbon systems, such as ethane, benzene and butadiene. The extended Huckel method developed by Roald Hoffman is the basis of the Woodward-Hoffmann rules. The energies of extended conjugated molecules such as pyridine, pyrrole and furan that contain atoms other than carbon also known as heteroatoms had also been determined using this method. Huckel expressed the total π-electron of a conjugated hydrocarbon as $E_\pi = n\alpha + 2\beta \sum_{i=1}^{n/2} \lambda_i$ where α and β are constants and the eigenvalues pertain to a special so called "molecular graph" like ethylene, benzene, butadiene, cyclo-buta-di-ene, etc. For the sake of simplicity, the expression for E_π is given, when n is even. The only non-trivial part in the above formula for E_π is $2 \sum_{i=1}^{n/2} \lambda_i$. It reduces to graph energy provided $\lambda_{\frac{n}{2}} \geq 0 \geq \lambda_{\frac{n}{2}+1}$ [3].

The complete graph K_n has eigenvalues n – 1 and – 1 (n – 1 times). At one time it was thought that the complete graph K_n has the largest energy among all n vertex

graphs G, that is, $E(G) \leq 2(n-1)$ with equality if and only if $G = K_n$. But Godsil in the early 1980s constructed an example of a graph on n vertices whose energy exceeds $2(n-1)$. Graphs whose energy satisfies $E(G) > 2(n-1)$ are called hyperenergetic. If $E(G) \leq 2(n-1)$, G is called non-hyperenergetic. In this paper we study about the energy, distance energy of connected graphs and skew energy of connected digraphs with respect to its spanning trees and its chords.

2. IN THIS SECTION, WE DEFINE SOME BASIC DEFINITIONS OF GRAPH THEORY

Definition 2.1: A linear graph or simply a graph G (V, E) consists of a set of objects $V = \{v_1, v_2, v_3, ..., v_n\}$ called vertices, and another set, $E = \{e_1, e_2, e_3, ..., e_n\}$ whose elements are called edges, such that each edge e_k is identified with an unordered pair (v_i, v_j) of vertices.

Definition 2.2: A directed graph or a digraph G in short consists of a set of vertices $V = \{v_1, v_2, v_3, ..., v_n\}$, a set of edges $E = \{e_1, e_2, e_3, ..., e_n\}$, and a mapping Ψ that maps every edge onto some ordered pair of vertices (v_i, v_j). A digraph is also referred to as an oriented graph.

Definition 2.3: A graph is said to be connected if there is at least one path between every pair of vertices in G. Otherwise the graph is said to be disconnected. A null graph of more than one vertex is disconnected. A disconnected graph consists of two or more connected graphs. Each of these connected graphs is called a component. The graph given below is a disconnected graph with two components which are connected subgraphs.

Definition 2.4: A simple graph in which there exists an edge between every pair of vertices is called a complete graph. The complete graph with n vertices is denoted by K_n. A complete graph is also referred as a universal graph or a clique. Since every vertex is joined with every other vertex through one edge, the degree of every vertex is $n-1$ in a complete graph of n vertices. Also the total number of edges in G is $\frac{n(n-1)}{2}$.

Definition 2.5: A graph G is said to be a bipartite graph, if there is a partition of V (G) into two subsets A and B such that no two vertices in the same subset are adjacent. If G is a bipartite graph with A and B as defined above, then [A, B] is called a bipartition of G; and G is denoted by G [A, B].

A bipartite graph G [A, B] is called a complete bipartite graph if every vertex in A is adjacent with every vertex in B. If and $|A| = m$ and $|B| = n$, then the graph is denoted by $K_{m, n}$.

Definition 2.6: A closed walk in which no vertex (except the initial and final vertex) appears more than once is called a circuit. That is, a circuit is a closed non-intersecting walk.

Definition 2.7: A tree is a connected graph without any circuits. A tree has to be a simple graph that is having neither a self-loop nor parallel edges. A graph with atleast one vertex is also a tree. A null tree is a tree without any vertices. The genealogy of a family can be represented by means of a tree. A river with its tributaries and sub-tributaries can be represented by a tree. Trees with two and three vertices are given below.

Definition 2.8: A tree T is said to be a spanning tree of a connected graph G if T is a subgraph of G and T contains all vertices of G. A spanning tree is also referred as a skeleton or scaffolding of G. Since spanning trees are the largest trees with maximum number of edges in G, it is also called as the maximal tree subgraph or maximal tree of G. The spanning trees K_3 of are given below:
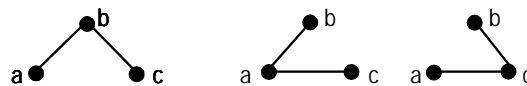
Definition 2.9: An edge in a spanning tree T is called its branch. An edge of G which is not in the given spanning tree is called a chord. Branches and chords are defined only with respect to a given spanning tree. An edge that is a branch of one spanning tree in a graph may be a chord with respect to another spanning tree.
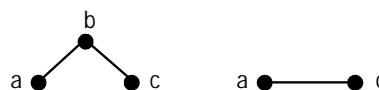
The edges {a, b} and {b, c} are the branches of the spanning tree of the complete graph K_3.

The edge {a, c} which is not in the spanning tree is a chord.

Definition 2.10: The union of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is another graph G_3 written as $G_3 = G_1 \cup G_2$ whose vertex set $V_3 = V_1 \cup V_2$ and the edge set $E_3 = E_1 \cup E_2$. The union operation is commutative. That is, $G_2 \cup G_1 = G_1 \cup G_2$. A connected graph G can be expressed as the union of two subgraphs T and $\bar{\tau}$ that is $G = T \cup \overline{T}$, where T is a spanning tree, and $\overline{T}$ is the complement of G in T. The graph $\overline{T}$ is the collection of chords, is called as the chord set or the tie set or the co-tree of T. It is also known that a connected graph of n vertices and e edges has n – 1 tree branches and e – n + 1 chords, with respect to any of its spanning trees.

3. IN THIS SECTION WE DISCUSS ABOUT THE BASIC DEFINITIONS OF ENERGY, DISTANCE ENERGY OF CONNECTED GRAPHS AND ALSO THE SKEW ENERGY OF CONNECTED DIGRAPHS

Definition 3.1: Let G be a simple, finite, undirected graph with n vertices and m edges. Let $A = (a_{ij})$ be the adjacency matrix of graph G. The eigenvalues of $\lambda_1, \lambda_2, ..., \lambda_n$ of A, assumed in non-increasing order, are the eigenvalues of the graph G. The energy of a graph G, denoted by E (G) is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. The set $\{\lambda_1, \lambda_2, ..., \lambda_n\}$ is the spectrum of G and is denoted by G. If the distinct eigenvalues of G are $\mu_1 > \mu_2 > ... > \mu_n$ and if their multiplicities are $m(\mu_1), m(\mu_2), ..., m(\mu_s)$ then we write

$$\text{Spec } G = \begin{pmatrix} \mu_1 & \mu_2 & .. & .. & \mu_s \\ m(\mu_1) & m(\mu_2) & .. & .. & m(\mu_s) \end{pmatrix}$$

Spec G is independent of labeling of the vertices of G. A is a real symmetric matrix with zero trace, these eigenvalues are real with sum equal to zero.

Definition 3.2: Let G be a simple graph with n vertices and m edges. Let G be also connected and let its vertices be labeled as $v_1, v_2, ..., v_n$. The distance matrix of a graph G is defined as a square matrix $D = D(G) = (d_{ij})$ where d_{ij} is the distance between the vertices v_i and v_j in G. The eigen values of the distance matrix D (G) are denoted by $\mu_1, \mu_2, ..., \mu_n$ and are said to be the D-eigenvalues of G. Since the distance matrix is symmetric, its eigenvalues are real and can be ordered as $\mu_1 \geq \mu_2 \geq ... \geq \mu_n$ and are said to form the D-spectrum of G.

The distance energy or the D-energy of a graph G, denoted by E_D or $E_D(G)$ is defined as $E_D = \sum_{i=1}^{n} |\mu_i|$ and it was first introduced by Indulal et al.

Definition 3.3: Let D be a simple digraph of order n with the vertex set $V(D) = \{v_1, v_2, ..., v_n\}$ and arc set $\Gamma(D) \subset V(D) \times V(D)$. We have $(v_i, v_i) \neq \Gamma(D)$ for all i, and $(v_i, v_j) \in \Gamma(D)$ implies that $(v_j, v_j) \notin \Gamma(D)$. The skew-adjacency matrix of the digraph D is the $n \times n$ matrix $S(D) = (s_{ij})$ where $s_{ij} = 1$, whenever $(v_i, v_j) \in \Gamma(D)$, $s_{ij} = -1$, whenever $(v_j, v_i) \in \Gamma(D)$, and $s_{ij} = 0$ otherwise. $S(D)$ is also the skew-symmetric matrix. The eigenvalues $\{\lambda_1, \lambda_2, ..., \lambda_n\}$ of $S(D)$ are all purely imaginary numbers and the singular values of $S(D)$ coincide with the absolute values $\{|\lambda_1|, |\lambda_2|, ..., |\lambda_n|\}$ of its eigenvalues. Consequently the energy of $S(D)$, which is defined as the sum of its singular values [1], is also the sum of the absolute values of its eigenvalues. This energy is called as the skew energy of the digraph D, denoted by $E_s(D)$. Therefore the skew-energy of a digraph is defined as $E_s(D) = \sum_{i=1}^{n} |\lambda_i|$.

Theorem 3.4: The energy of connected graph G decreases with respect to the sum of the energies of its spanning tree and the chord. That is

$$E(G) < E(T) + E(\overline{T}).$$

Proof: Let G be any connected graph with vertices and edges.

Let T and $\overline{T}$ be its spanning tree and chord.

Jane Day and Wasin So have shown that with deletion of an edge in a connected graph G, the energy of connected graph G increases, decreases or remains the same.

A connected graph G of n vertices has n – 1 branches and e – n + 1 chords.

The spanning tree T has n – 1 edges and the chord $\overline{T}$ has e – n + 1 edges.

Since the number of edges of the spanning tree T and the chord $\overline{T}$ is less than that of the connected graph G, the energy of the spanning tree T is either less than or greater than or equal to that of the connected graph G.

It is seen that in all the connected graphs G, the energy of the chord $\overline{T}$ is less than that of the energy of the connected graph G.

But the sum of the energies of the spanning tree T and the chord $\overline{T}$ of the connected graph G is greater than that of the energy of the connected graph G except for the star graph.

That is the energy of the connected graph G decreases with respect to the sum of the energies of any of its spanning tree and the chord.

We show that the above statement is true for different types of connected graphs.

Case 1: Let be the complete graph K_n.

We know that a connected graph G of n vertices and e edges has n − 1 tree branches and e − n + 1 chords with respect to any of its spanning tree.

Jane Day and WasinSo have shown that the deletion of an edge in a complete graph K_n decreases its energy. That is $E(K_n) > E(K_n − \{e\})$.

We know that the number of spanning trees of the complete graph is n^{n-2}.

The chord $\overline{T}$ of the complete graph K_n is a disconnected graph with some null vertices.

Since the number of edges of the spanning tree and chord of the complete graph K_n is less than n, the energies of the spanning tree and the chord of the complete graph K_n is less than that of the energy of the complete graph K_n.

Case 2: Let G be the cycle C_n of length K_n.

We know that a cycle is possible from a connected graph with n vertices and m edges if and only if $m \geq n$.

The energy of any spanning tree of the cycle C_n is either less than or greater than that of the energy of the cycle C_n. The complement $\overline{T}$ of the spanning tree T of C_n is a complete graph K_2, whose energy is 2. That is $E(\overline{T}) = 2$.

Case 3: (i) Let G be only the bipartite graph $K_{m,n}$.

If G is a bipartite graph with n > 2 vertices and $m \geq \frac{n}{2}$ edges, then the energy

of the bipartite graph is defined as $E(G) \leq 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left(2m - 2\left(\frac{2m}{n}\right)^2\right)}$

and the equality case is characterized in some special cases [15].

The energy of a graph as a function of its m number of edges satisfies

$2\sqrt{m} \leq E(G) \leq 2m$ where the equality on the left holds if and only G is a complete bipartite graph and on the right holds if and only if G is a matching of m edges [3].

The energy of any spanning tree T of the bipartite graph $K_{m,n}$ is seen to be less than that of the energy of the bipartite graph $K_{m,n}$.

The complement of the spanning tree T of the bipartite graph $K_{m,n}$ is always a disconnected graph. This disconnected graph is the union of the complete graphs K_2 and some isolated vertices. The energy of the chord $\overline{T}$ is sum of

the energies of the disconnected components. Since the energy of the complete graph K_2 is a multiple of 2, the energy of the chord $\overline{T}$ is also a multiple of 2.

(ii) Let G be the complete bipartite graph $K_{m,n}$.

We know that for the complete bipartite graph, $E(K_{m,n}) = 2\sqrt{m}$ where m is the number of edges.

The energy of any spanning tree T of the complete bipartite graph $K_{m,n}$ is less than that of the energy of the complete bipartite graph $K_{m,n}$. The complement of the spanning tree T of the complete bipartite graph $K_{m,n}$ is a disconnected graph with some isolated vertices. The energy of is the sum of the energies of $\overline{T}$ its disconnected components.

(iii) Let G be the complete regular bipartite graph $K_{n,n}$.

We know that the energy of the complete regular bipartite graph $K_{m,n}$ is 2n.

The energy of a complete regular bipartite graph increases with deletion of an edge from it.

That is $E(K_{n,n}) < E(K_{n,n} - \{e\})$.

The energy of the spanning tree T of the regular complete bipartite graph $K_{n,n}$ is greater than that of the energy of the complete bipartite graph $K_{n,n}$. The complement of the spanning tree T of the regular complete bipartite graph $K_{n,n}$ is a disconnected graph. The energy of $\overline{T}$ is the sum of the energies of its disconnected components.

Case 4: Consider the star graphs.

Consider the star graphs $K_{1,n-1}$.

We know that a star graph and its edge deleted graph are complete bipartite graphs.

The star graph $K_{1,n-1}$ uniquely has the smallest energy among all graphs with n vertices where none of the n vertices are isolated [3].

The energy of the star graph is defined as $E(K_{1,n-1}) = 2\sqrt{n-1}$ [3].

Every star graph is itself a spanning tree.

The energies of the star graph $K_{1,n-1}$ and its spanning tree T are same. That is $E(K_{1,n-1}) = E(T)$.

Also the chord of the star graph $K_{1,n-1}$ is a null graph.

This implies that the energy of the co-tree is zero. That is $E(\overline{T}) = 0$. Therefore we have

$$E(K_{1, n-1}) = E(T) + E(\overline{T}) \quad \text{or} \quad E(K_{1, n-1}) = E(T).$$

In all the cases, we find that the energy of the connected graph G to be less than or equal to the sum of the energies of the spanning tree T and the chord $\overline{T}$ of the connected graph G.

That is $E(G) < E(T) + E(\overline{T})$.

Theorem 3.5: The distance energy of a connected graph is always less than that of its spanning tree.

That is $E_D(G) < E_D(T)$.

Proof: Let G be the connected graph and T be its spanning tree.

The distance energy of a connected graph G is greater than or equal to $\sqrt{n(n-1)}$, where n is the number of vertices [18].

The distance energy of the complete graph is same as that of the energy of the complete graph K_n.

That is $E_D(K_n) < E(K_n)$.

The distance energy of the complete bipartite graph $K_{m, n}$ is given by

$$E_D(K_{m, n}) = 4(m + n - 2) \text{ for } m, n \geq 2 \text{ [19]}.$$

The distance energy of a connected graph G always less than or equal to its edge deleted graph.

Since the number of edges in a spanning tree T of any connected graph is n – 1, the distance energy of the spanning tree T of any connected graph G will be greater than the distance energy of the connected graph. The distance energy of the chord $\overline{T}$ of connected graphs like complete graphs, bipartite graphs cannot be found as the chord graphs are all disconnected graphs. In case of star graphs, the chord graph is a null graph.

Theorem 3.6: The skew energy of connected digraph G decreases with respect to the sum of the skew energies of its spanning trees and the chords.

That is $E_s(G) < E_s(T) + E_s(\overline{T})$.

Proof: Let G be the connected digraph. Let T be the spanning tree of the digraph G, and let $\overline{T}$ be the chord of the connected digraph G.

The skew energy of the directed tree is same as that of the energy of the undirected tree [1].

We can say that the skew energies of the spanning directed tree T and the energy of the spanning undirected tree T are same.

The complement $\overline{T}$ of the directed tree T of the connected digraph G is a disconnected digraph with some isolated vertices.

The skew energy of the disconnected digraph is the sum of the skew energies of its disconnected components.

The skew energy of the connected digraph G is seen to be less than that of the sum of the skew energies of the spanning tree T and the co-tree $\overline{T}$. Therefore we can say that $E_S(G) < E_S(T) + E_S(\overline{T})$.

We can verify the above two theorems with the examples of some connected graphs and connected digraphs with respect to one of its spanning trees and chord given in tabular form.

Conceted graph G	E (G)	E (T)	E ($\overline{T}$)	E_D (G)	E_D (T)	E_S (G)	E_S (T)	E_S ($\overline{T}$)
K_3	4.000	2.828	2.000	4.000	5.464	3.464	2.828	2.000
K_4	6.000	4.472	4.472	6.000	10.325	5.656	4.472	4.472
C_3	4.000	2.828	2.000	4.000	5.464	3.464	2.828	2.000
C_4	4.000	4.472	2.000	8.000	10.324	5.656	4.472	2.000
C_5	4.472	5.464	2.000	12.000	16.576	6.156	5.464	2.000
$K_{2,3}$	4.898	5.226	2.828	10.671	14.919	6.828	5.226	2.828
$K_{2,3}$	5.596	5.226	2.000	13.076	14.919	6.293	5.226	2.000
$K_{3,4}$	8.120	7.880	4.000	27.401	29.728	8.120	7.880	4.000
$K_{2,2}$	4.000	4.472	2.000	8.000	10.325	4.000	4.472	2.000
$K_{1,4}$	4.000	4.000	0.000	13.212	13.212	4.000	4.000	0.000

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