On the Energy of Certain Recursive Structures

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Abstract

Eigenvalues of a graph are the eigenvalues of its adjacency matrix. The multiset of eigenvalues is called the *spectrum*. The energy of a graph is the sum of the absolute values of its eigenvalues. In this paper, we devise an algorithm which generates the adjacency matrix of WK - recursive structures $WK(3, L)$ and $WK(4, L)$ and use it in the effective computation of spectrum and energy.

1 INTRODUCTION

Spectral methods in graph theory have received great attention since their introduction and have proved to be a valuable tool for the theoretical and applied graph theory [1, 2]. The study of graph eigenvalues realizes increasingly rich connections with many other areas of mathematics. A particularly important development is the interaction between spectral graph theory and differential geometry. Spectral graph theory has a long history. In the early days, matrix theory and linear algebra were used to analyse adjacency matrices of graphs. Algebraic methods are especially effective in

treating graphs which are regular and symmetric. Sometimes, certain eigenvalues have been referred to as the algebraic connectivity of a graph. There is an interesting analogy between spectral Riemannian geometry and spectral graph theory. The concepts and methods of spectral geometry bring useful tools and crucial insights to the study of graph eigenvalues, which in turn lead to new directions and results in spectral geometry. New spectral techniques have emerged and they are powerful and well-suited for dealing with general graphs. In a way, spectral graph theory has entered a new era.

A graph G with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ can be represented by its adjacency matrix $A = A(G) = [a_{ij}]$ where $a_{ij} = 1$ if v_i and v_j are adjacent and $a_{ij} = 0$ otherwise. The spectrum of G is the set of numbers which are eigenvalues of $A(G)$, together with their multiplicities. If the distinct eigenvalues of $A(G)$ are $\lambda_1 > \lambda_2 > \ldots > \lambda_s$ and their multiplicities are $m(\lambda_1), m(\lambda_2) \ldots m(\lambda_s)$ then we can write the spectrum as

There are many properties which can be explained using the spectrum like energy, connectedness, vertex connectivity, chromatic number, and perfect matching etc. It is one of the most important algebraic invariants of a graph. Let $d(v)$ denote the degree of $v \in V(G)$ and let $D = D(G)$ be the diagonal matrix indexed by $V(G)$ and with $D_{vv} = d(v)$. The matrix $L = D - A$ and $Q = D + A$ are called the Laplacian and Signless Laplacian matrices respectively.

The energy $E(G)$ of a simple graph G is defined to be the sum of the absolute values of the eigenvalues of G. In [3] the spectra and energy of several classes of graphs containing a linear polyene fragment are obtained. In [4] the energy of iterated line graphs of regular graphs and in [5] the energy of some self-complementary graphs is discussed. The energy of regular graphs is discussed in [6]. Some works pertaining to the computation of energy can be seen in [7, 8, 9, 10, 11].

The aim of this section is to draw the attention of the mathematical community to rapidly growing applications of the theory of graph spectra and energy of graphs. There are applications of graph eigenvalues in Computer Science in various investigations. There are also applications in several other fields like biology, geography, economics and social sciences.

Motivation for founding the theory of graph spectra has come from applications in chemistry and physics. The first mathematical paper on graph spectra was motivated by the membrane vibration problem [12]. In quantum chemistry, the skeleton of a non-saturated hydrocarbon is represented by a graph. The energy levels of the electrons in such a molecule are the eigenvalues of the graph. The stability of molecules is closely related to the spectrum of its graph [13]. The spectra of graphs, or the spectra of

certain matrices which are closely related to adjacency matrices appear in a number of problems in statistical physics (see, for example, [14, 15, 16]). Graph spectra appear in internet technologies, pattern recognition, computer vision, and in many other areas.

The eigenvalues of a graph characterize the topological structure of the graph. The technique is usually efficient in counting structures, e.g., acyclic digraphs, spanning trees, Hamiltonian cycles, independent sets, Eulerian orientations, cycle covers, k-colorings etc. [17]. If a graph possesses certain properties, using its eigen-properties it is possible to derive (recurrence) formulas for counting the number of structures.

In this paper, we devise an algorithm which generates the adjacency matrix of the recursive structures $WK(3, L)$ and $WK(4, L)$. This algorithm works efficiently in software platforms like Maple, Matlab etc. Once the algorithm generates the adjacency matrix, then there are inbuilt functions in the software to calculate the eigenvalues and hence the energy.

2 WK-RECURSIVE STRUCTURES

The architecture of the WK-recursive networks denoted by $WK(K, L)$ [18] depends on the equality between the amplitude W and the degree K of virtual nodes and L the expansion level. The first level virtual node is constructed by connecting K real nodes of degree K to each other in a "fully connected configuration", and leaving K links free. Therefore, a virtual node is virtually similar to real node of degree K. By the same manner, K first level virtual nodes may be used to construct a second level virtual node, also of degree K, and so on, until level L, which may be constructed from K,$(L-1)^{th}$ level virtual nodes. Amplitude W of the L^{th} level virtual node is the number of its $(L-1)^{th}$ level virtual nodes, having of course $W = K$. The WK-recursive topologies are identified essentially by the following analytic relation $L = log_K N$ where N is the number of real nodes, K is the node degree and L is the expansion level. In the WK-recursive graph $WK(K, L)$, there are K corner real nodes of degree $(K-1)$. Therefore, the edge connectivity, which is the smallest number of links that can be deleted in order to disconnect the graph, is equal to $(K-1)$. The node connectivity of the graph is the smallest number of nodes that can be deleted in order to disconnect the graph and is also equal to $(K-1)$. The diameter of the WK-recursive topologies is $D = 2^L - 1$. In general, the diameter depends only on the expansion level whatever the node degree is. $WK(K, L)$ is a recursive structure. It consists of K copies of $WK(K, L-1)$ or K^2 copies of $WK(K, L-2)$ and so on. Thus, $WK(K, L)$ contains K^{L-1}

copies of $WK(K,1)$.

2.1 Labelling Algorithm

In order to generate the adjacency matrix of the recursive network $WK(3,L)$ we propose a specific labelling method. We call this labelling as WK labelling.

Algorithm *WK Labelling*

Input: $WK(K,L)$ with K attached copies of $WK(K,L-1))$ denoted by $W_1^{L-1}, W_2^{L-1}, \ldots, W_K^{L-1}$.

Step 1: Label $WK(K,1)$ in the anti-clockwise sense.

Step 2: At stage t, $W_1^{t-1} \simeq WK(K,t-1)$. The unlabelled vertices of W_i^{t-1} , $2 \leq i \leq K$ induce a graph isomorphic to $WK(K,t-1)$. Let $y = |V(WK(K,t-1))|$. Label an unlabelled vertex of W_i^{t-1} , $1 \leq i \leq K$ as $j+(i-1)y$ if the corresponding vertex in W_1^{t-1} is labelled j.

Step 3: Stop when step 2 cannot be implemented further.

Output: *WK Labelling* of $WK(K,L)$

Proof of correctness of $WK3$ labelling: We observe that the above algorithm is proper since each vertex in $WK(K,L)$ receives a unique label, as at every stage of the algorithm only the unlabelled vertices are labelled.

We now propose an algorithm to generate the adjacency matrix of $WK(3,L)$. The adjacency matrix of $WK(3,L)$ is a $3^L \times 3^L$ matrix. Finding the adjacency matrix becomes difficult as L increases. In this algorithm, we provide a technique to compute the adjacency matrix for any L using the adjacency matrix of $WK(3,1)$ which is the smallest substructure of $WK(3,L)$. The algorithm is as follows:

2.2 Algorithm *Adjacency* $WK3$

Input: Adjacency matrix A_1 of $WK(3,1)$, dimension L, $k=1$.

Step 1: $A_L$is a $3^L \times 3^L$ matrix all of whose diagonal entries are A_1 and zeros elsewhere.

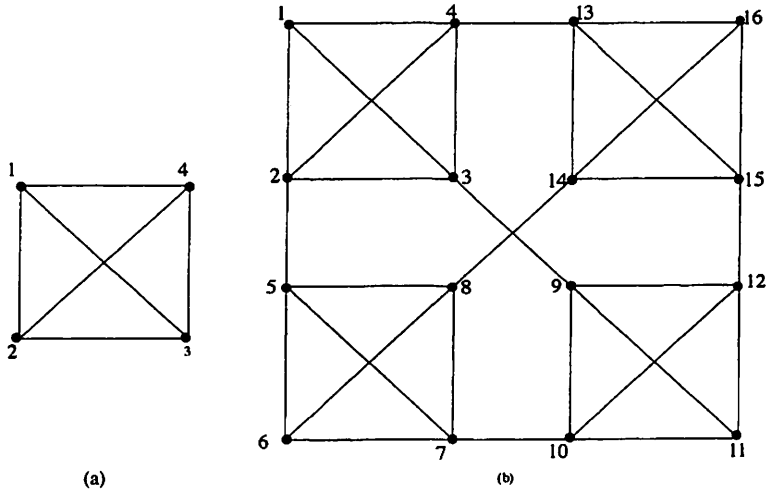

Figure 1: Labelling of (a)$WK(4,1)$ (b)$WK(4,2)$ using WK labelling algorithm

Step 2: $k = k + 1$,

$$y = y(k) = 1 + \sum_{l=2}^{k} 3^{l-2}$$

Step 3: At stage k of the algorithm, for $m = 0, 1, 2...3^{L-k} - 1$

Put $A_k(y + m3^k, 2y + m3^k) = 1$

$A_k(2y + m3^k, y + m3^k) = 1$

$A_k(4y - 2 + m3^k, 5y - 2 + m3^k) = 1$

$A_k(5y - 2 + m3^k, 4y - 2 + m3^k) = 1$

$A_k(2y - 1 + m3^k, 4y - 1 + m3^k) = 1$

$A_k(4y - 1 + m3^k, 2y - 1 + m3^k) = 1$

Step 4: If $k < L$, Go to Step 2.

Step 5: Stop

Proof of Correctness of Algorithm *Adjacency1* $WK3$:

In Step 1 of the algorithm, 3^L edges of $WK(3, L)$ are accounted for. In the first iteration of Step 3 (i.e. when $k = 2$), $3 \times (3^{L-2})$ edges are accommodated and in its i^{th} iteration $3 \times (3^{L-i})$. Step 3 is repeated $(L-1)$

times. Therefore Step 3 accommodates a total of $(3^L - 3)/2$ edges. Hence the total number of edges accounted by this algorithm is $(3^{L+1} - 3)/2$, which is the total number of edges of $WK(3, L)$.

We next propose an algorithm to generate the adjacency matrix of $WK(4, L)$.

2.3 Algorithm *Adjacency* $WK4$

The adjacency matrix of $WK(4, L)$ is a $4^L \times 4^L$ matrix. In this algorithm, the adjacency matrix of $WK(4, L)$ for any L is obtained using the known adjacency K of $WK(4, 1)$. The algorithm is as follows:

Input: Adjacency matrix A_1 of $WK(4,1)$,dimension L, $k = 1$

Step 1: A_l is a $4^L \times 4^L$ matrix all of whose diagonal entries are A_1 and zeros elsewhere.

Step 2: $k = k + 1$

$$y = y(k) = 1 + \sum_{l=2}^{k} 4^{l-2}$$

Step 3: At stage k of the algorithm, for $m = 0, 1, 2...4^{L-k} - 1$

Put $A_k(y + m4^k, 3y - 1 + m4^k) = 1$

$A_k(3y - 1 + m4^k, y + m4^k) = 1$

$A_k(2y - 1 + m4^k, 6y - 3 + m4^k) = 1$

$A_k(6y - 3 + m4^k, 2y - 1 + m4^k) = 1$

$A_k(3y - 2 + m4^k, 9y - 5 + m4^k) = 1$

$A_k(9y - 5 + m4^k, 3y - 2 + m4^k) = 1$

$A_k(10y - 6 + m4^k, 6y - 4 + m4^k) = 1$

$A_k(6y - 4 + m4^k, 10y - 6 + m4^k) = 1$

$A_k(9y - 6 + m4^k, 11y - 7 + m4^k) = 1$

$A_k(11y - 7 + m4^k, 9y - 6 + m4^k) = 1$

$A_k(5y - 3 + m4^k, 7y - 4 + m4^k) = 1$

$A_k(7y - 4 + m4^k, 5y - 3 + m4^k) = 1$

Step 4: If $k < L$, Go to Step 2.

Step 5: Stop

Proof of Correctness of Algorithm *Adjacency* $WK4$:

In Step 1 of the algorithm, $4^L \times 6$ edges of $WK(4, L)$ are accounted for. In the first iteration of Step 3 (i.e. when $k = 2$), $6 \times (4^{L-2})$ edges are accommodated and its i^{th} iteration $6 \times (4^{L-i})$ edges. Step 3 is repeated $(L-1)$ times. Therefore Step 3 accommodates a total of $2(4^{L-1}-1)$ edges. Hence the total number of edges accounted by this algorithm is $2(4^L - 1)$, which is the total number of edges of $WK(4, L)$.

3 CONCLUSION

The algorithm proposed in this paper can be simulated using any of the mathematical packages like MATLAB, Maple or Mathematica. The adjacency matrix thus obtained from the algorithm is directly used to obtain the spectrum. From the adjacency matrix generated , Laplacian and Signless Laplacian matrices are also obtained and hence their respective energies.

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