LAPLACIAN SPECTRUM, EFFECTIVE RESISTANCE AND ROBUSTNESS IN ELECTRICAL NETWORK OF FULLERENE C_{60}

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In this work, the Laplacian spectrum of some well-known graphs such as fullerene C_{60} and hyper cubes is computed. Using the Laplacian spectrum, the effective graph resistance of these graphs, as a network, is given.

(Received April 9, 2013; Accepted May 31, 2013)

Keywords: Effective resistance, Electrical network, Caylay graph.

1. Introduction

Effective resistances in regular electrical networks, where currents voltages and resistances are scalar valued, have been known to have far reaching implications in a variety of problems. Recurrence and transience in random walks in infinite networks [1] and the coverage and commute times of random walks in graphs [2] are determined by this effective resistance. There is a strong connection between variance of the estimate of a scalar valued variable from relative measurements defined on a graph and effective resistance, which was discovered by Karp *et al.* [3]. It was later shown by Barooah and Hespanha [4] that this analogy can be extended to vector measurements with matrix-valued covariances with the introduction of generalized electrical networks, with matrix-valued currents, voltages, and resistances.

Let us recall some notations introduced in [5]. Let G be a connected graph with $V(G) = \{1,2,\ldots,n\}$ vertex set. The shortest path distance $d(i,j)$ between the vertices i and j is the classical notion of distance and is extensively studied. However, this concept of distance is not always appropriate. Another notion of distance, called "resistance distance" defined in [6], in view of an interpretation of the notion vís-a-vís resistance in electrical networks, captures the notion of distance in terms of communication more appropriately. Resistance distance is mathematically more tractable, as well. Furthermore, in the case of a tree, resistance distance and classical distance coincide.

There have been two important recent trends in both military and civilian communications. The first is network-centric operation, which bases organizational activity strongly around an internal network. In the civilian sphere, this is called e-commerce (and, in more recent developments, m-commerce). In the military sphere, this is called Network Centric Warfare (NCW) [7].

The second trend is the increasing threat to communications infrastructure. In the civilian sphere, the threat is from terrorist attacks, while in the military sphere this comes from the increasing tendency to view communications networks as high-value targets.

The first trend makes networks more important, while the second makes them more vulnerable. This dilemma makes it critically important to address network robustness, i.e. the continued ability of the network to perform its function in the face of attack.

Dekker and Colbert [8] specifically focused on the robustness of the network topology. They used graph theory to investigate which network topologies are the most robust. Graph theory

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provides two different measures of connectivity which are possible ways of measuring robustness, and it is showned that node connectivity is the most useful of these. They examined the relationship between node connectivity and the degree of symmetry of the network, and they suggested that it is important for robust networks to satisfy two conditions; node-similarity and optimal connectivity.

2. Theory

Resistance distance admits several equivalent definitions. Let G be a connected graph with vertex-set V(G)={1,2,…,n} and edge-set E(G)={e_1,e_2,…,e_m}. The Laplacian matrix of G, denoted by L(G), is the n×n matrix defined as follows. The rows and columns of L(G) are indexed by V(G). If i≠j then the (i,j)-entry of L(G) is 0 if vertex i and j are not adjacent, and it is -1 if i and j are adjacent. The (i,i)-entry of L(G) is d_i; the degree of the vertex i, i = 1,2,..,n. The resistance distance between vertices i and j defined as r(i,j)=det L(i,j|i,j)/det L(i,i) where L(i,j|i,j) and L(i,i) denote the submatrix of L(G) obtained by deleting the rows and columns {i,j} and {i} respectively (See [5]).

If x is a vector of order n×1 then the norm ||x|| is defined to be the usual Euclidean norm; $||x|| = (\sum x_i^2)^{1/2}$. We interpret the resistance distance between the two vertices i and j in terms of an "optimal" flow from i to j. First we give some definitions. Let the edges of G be assigned an orientation and let Q be the vertex-edge incidence matrix. Denote by e_{ij} the n×1 vector with the ith coordinate equal to 1; the jth coordinate equal to -1; and zeros elsewhere. A unit flow from i to j is defined [5] as a function f : E(G)→R such that

$$Q[f(e_1),f(e_2),\ldots,f(e_m)]^t=e_{ij}.$$

The interpretation of the above equation is easy; at each vertex other than i, j the incoming flow is equal to the outgoing flow; at i the outgoing flow is 1 whereas at j; the incoming flow is also 1. The norm of a unit flow *f* is defined to be

$$||f||=(\sum f(e_j)^2)^{1/2}.$$

r(i,j) is the minimum value of $||f||^2$ where ||f|| is a unit flow from i to j (See [5], p.115).

There is a close connection between the interpretation of r(i,j) based on electrical networks, which we discuss below.

Let G be a connected graph with V(G) = {1,2,…,n}, and let i,j be two vertices and i≠j. We think of G as an electrical network in which a unit resistance is placed along each edge. Current is allowed to enter the network only at vertex i and leave it only at j. Let v(k) denote the voltage at the vertex k. We set v(i) = 1 and v(j) = 0. By Ohm's law, the current flowing from x to y, where xy is an edge, is given by v(x)-v(y). According to Kirchhoff's law, at any point k, k≠i, j,

$$\sum_{y\in N[k]}(v(k)-v(y))=0$$

where N[k] denotes the set of all adjacent vertices of vertex k. It is easy to see that

$$v(k)=(-1)^{i+k}\,\frac{\det L(i,j\mid k,j)}{\det L(j\mid j)}$$

for k≠j and v(j)=0 (See [5], p.118). The current flowing into the network at vertex i is given by the sum of the currents from y to i for each $y\in N[i]$ and this equals

$$\sum_{y\in N[i]}(v(y)-v(i))=\sum_{y\in N[i]}v(y)-d_i.$$

Finally, the current flowing into the network is

$$\frac{\det L(j \mid j)}{\det L(i, j \mid i, j)}$$

which is precisely the reciprocal of r(i,j) (See [5], p.118). The reciprocal of the current is called the "effective resistance" between i, j and this justifies the term "resistance distance". Bollobás [15] and Doyle and Snell [16] are classical references for a graph theoretic treatment of resistance.
Let G be a graph with vertex set V(G)={1,2,…,n}. The *effective graph resistance* R_G is the sum of the e_ective resistances over all pairs of vertices in the graph G:

$$R_G = \sum_{1 \le i < j \le n} r(i, j) .$$

In the literature the efective graph resistance is also called total efective resistance or Kirchhof index. Klein and Randić [6] have proved that it can be written as a function of the non-zero Laplacian eigenvalues:

$$R_G = n\sum_{i=2}^{n} \frac{1}{\mu_i}$$

where $0=\mu_1\le\mu_2\le\ldots\le\mu_n$ are the eigenvalues of the Laplacian matrix L(G).

There are two concepts of connectivity for a graph G which can be used to model network robustness: node (vertex) and link (edge) connectivity denoted by κ(G) and λ(G) respectively. A graph has the vertex-(edge-) connectivity k if k is the least number of vertices (edges) which may be removed so that the remaining graph is disconnected or consists of an isolated vertex . These connectivity measures can be calculated using the maximum-flow algorithm [9]. It is well-known that $\kappa(G)\le\lambda(G)\le d_{min}(G)$ where $d_{min}(G)$ is the minimum degree of vertices of G (See [9], Theorem 2.9).

If $\kappa(G) = \lambda(G) = d_{min}(G)$ for some graph, we say that the graph is *optimally connected*, since the node and link connectivities are as high as possible, i.e. the network is as robust as it could be, given the value of $d_{min}(G)$. In [8] several strategies for designing optimally connected graphs are considered.

We say a graph is *regular* if every node has same degree. An *automorphism* of a graph is a permutation π of the nodes which preserves links. A graph is *node-similar* (vertex-transitive) if for any two nodes u and v there is an automorphism π such that $\pi a = b$. A graph is symmetric if for any two links ab and xy there is an automorphism π such that $\pi a = x$ and $\pi b = y$.

If a network is both node-similar and optimally connected, then it provides maximum resistance to node destruction. Let G be a connected node-similar regular graph of degree d. Then λ(G)=d, if d≤4, κ(G)=d (See [10]). As a sequence of this result fullerene C_{60} and trancated octahedral graphs are optimal connected with κ=λ=d=3. In the last section, we will consider these graphs as networks.

An alternative way of designing optimally connected graphs involves *group theory*, an area of abstract algebra with a long tradition. For more details and initial definitions relating group theory which are appeared in this paper, you can see [11]. Just mention that a group is a set containing an element e, and equipped a binary operation . such that for every element x there is an element denoted by x^{-1} that $x.x^{-1}=x^{-1}.x=e$. Also x.e=e.x and the operation . is associative.

Let H be a group and $S=S^{-1}$ be a subset of H\{e}. Then the graph Γ(H,S) with nodes H is called a *Cayley graph* if every link of this graph be of the form ab where b=a.s for some s in S. It is easy to see that a Cayley graph is regular of degree |S|, the size of S, and node-similar. Also in these graphs κ=λ=|S| (for more details see [12]). Hence The importance of minimal Cayley graphs for network design lies in the fact that they are optimally connected.

3. Results

As we saw in the previous section, graph-theoretic concepts of node connectivity and link connectivity as measures of network robustness, and argued that node connectivity is most appropriate for modelling the robustness of network topologies in the face of possible node destruction. This is important both for military networks and for civilian networks facing possible terrorist activity. The most robust networks are optimally connected, which means that the node connectivity is as high as possible, given the node degrees. Also we saw that Cayley graphs are optimally connected. In this section we consider some well-known Cayley graphs as networks and compute their effective graph resistances.

Representation theory of groups is a useful branch of group theory which help us to find the spectrum of adjacency matrix of the Cayley graphs (for more details see [13]). In the following examples we give directly the eigenvalues of considered graphs.

Since the Cayley graphs are regular we have the following theorem.

Theorem 1. Let $G=\Gamma(H,S)$ be a connected Cayley graph. Let $L(G)$ be the Laplacian matrix of G and $A(G)$ be its adjacency matrix. Then the eigenvalues of $L(G)$ are of the form $|S|-\alpha$ where α is an eigenvalue of $A(G)$, i.e

$$Spec(L(G)) = \{|S| - \alpha \mid \alpha \in Spec(A(G))\}$$

where Spec(X) is the multiset of all eigenvalues of matrix X.

Proof. Let $D(G)=[d_{ij}]$ where $d_{ij}=d_i$ when i=j and is 0 when $i\neq j$. Clearly $L(G)=D(G)-A(G)$. Since G is regular of degree |S|, $D(G)=|S|I$ where I is the identity matrix. Now by Cayley-Hamilton Theorem (See [5]) the result is clear.

Example 1. Truncated Octahedron G is a Cayley graph on the group S_4, the symmetric group on 4 letters, with 24 nodes, Fig.1. This graph is 3-regular and $Spec(A(G))=\{(\pm3)^{[1]}, (\pm1)^{[3]}, (\pm1\pm\sqrt{2})^{[3]}, (\pm\sqrt{3})^{[2]}\}$ where $\alpha^{[k]}$ means α is an eigenvalue with multiplicity k (See http://mathworld.wolfram.com/TruncatedOctahedron.html). Hence $Spec(L(G))=\{0^{[1]}, 6^{[1]}, 2^{[3]}, 4^{[3]}, (2\pm\sqrt{2})^{[3]}, (4\pm\sqrt{2})^{[3]}), (3\pm\sqrt{3})^{[2]}\}$ and $R_G=24(149/12)=298$. Also as we saw before $\lambda(G)=\kappa(G)=3$.

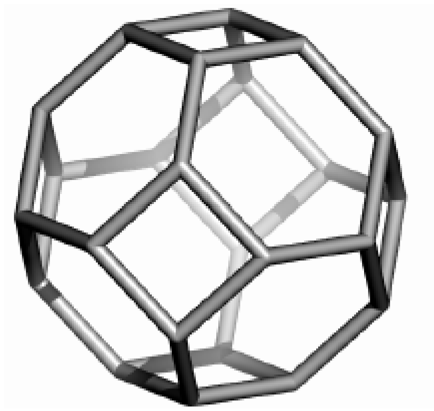

Fig.1. Truncated Octahedron

Example 2. The fullerene graph C_{60} is a Cayley graph on A_5, the alternating group on 5 letters, Fig.2. Let us denote this graph with Γ. This graphs is a 3-regular graph with 60 nodes. Using the representations of the group A_5, we can say the eigenvalues of the adjacency matrix of Γ are roots of the following equations (for more details see [14], page 119. Note that you should put t=1):

$(x^2+x-1)(x^3-2x^2-2x+3)=0$ with multiplicity 5,

$(x^2+x-2)(x^2+x-4)=0$ with multiplicity 4,

$(x^2+3x+1)(x^4-3x^3-2x^2+7x+1)=0$ with multiplicity 3,

x-3=0 with multiplicity 1.
By solving the above equations, the spectrum of adjacency matrix of Γ is 3[1], 1[9], (-2)[4],
$(\frac{-1\pm\sqrt{5}}{2})^{[5]},(\frac{1\pm\sqrt{13}}{2})^{[5]},(\frac{-1\pm\sqrt{17}}{2})^{[4]},(\frac{-3\pm\sqrt{5}}{2})^{[3]}, (\pm\sqrt{\frac{\sqrt{5}+19}{8}}+\frac{3-\sqrt{5}}{4})^{[3]},(\pm\sqrt{\frac{19-\sqrt{5}}{8}}+\frac{3+\sqrt{5}}{4})^{[3]}$.
Hence, by Theorem 1, $R_G = \frac{46612}{19}$.

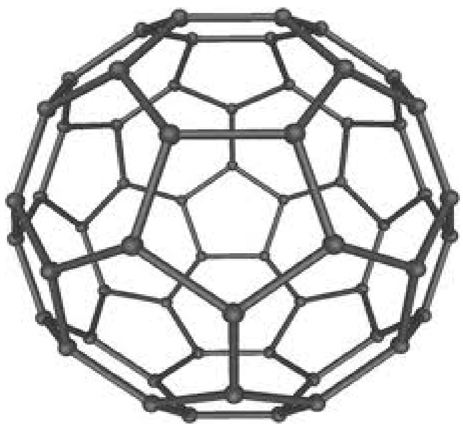

Fig.2. Fullerene C_{60}.

Example 3. The *Hamming graph H(q,m)* is the graph whose nodes are all the vectors $a=(a_1, \ldots, a_q)$ with a_i are in tigers in $\{0, \ldots, m-1\}$, and with links between vectors that differ in exactly one position, i.e. with a Hamming distance of 1, Fig.3. Note that H=H(q,2) is the q-dimensional hypercube. H(q,2) is a q-reqular and a Cayley Graph with adjacency eigenvalues q-2w_H(a) where w_H(a) is the number of nonzero coordinates in a (for more details see [13]). So $Spec(A(H)) = \{q - \binom{q}{k} \mid k = 0,1,\ldots,q\}$. Hence λ(H)=κ(H)=q and $R_H = q^2 \sum_{k=1}^{q} 1/\binom{q}{k}$.

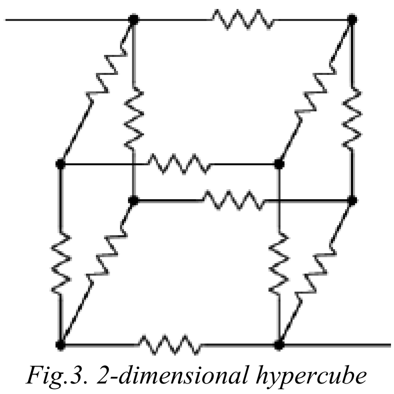

Fig.3. 2-dimensional hypercube

Acknowledgement

This paper supported by the Islamic Azad University, Majlesi Branch.

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