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A NEW APPROACH IN BEHAVIORAL SCIENCES USING CORRELATION BETWEEN ENERGY OF FULLERENES

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The energy of a square matrix associated a graph is defined to be the sum of the absolute values of average derivation of mean of its eigenvalues. The energy of adjacency matrix of graph is called the energy of graph and the energy of the distance matrix is called, distance energy of it. We compute the energy and distance energy of fullerene graphs and check the behavior and correlation between them.

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1. Introduction

Let G = (V,E) be a simple graph with n vertices and A(G) be the (0,1)-adjacency matrix of G. It is well-known fact that A(G) is symmetric and its eigenvalues are real. Without loss of generality we can write them as $\lambda_1(G) \geq \lambda_2(G) \geq ... \geq \lambda_n(G)$. The characteristic polynomial of G is just det(I – A(G)), denoted by $\phi(G,\lambda)$. The greatest eigenvalue $\rho = \lambda_1(G)$ is called the index (or spectral radius) of G [1]. If G is connected, then A(G) is irreducible and so it is well-known that $\lambda_1(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\lambda_1(G)$ by the Perron–Frobenius theory of non negative matrices. The energy of a graph [2-10] is defined to be the sum of the absolute values of its eigenvalues. This notion was introduced by Gutman and is related to the concept of the total-electron energy of a molecule in chemistry. A fullerene [11,12] is a molecule consisting entirely of carbon atoms. Each carbon is three-connected to other carbon atoms by one double bond and two single bonds. These molecules are of great importance in chemistry: Buckyball is one of famous fullerenes was named Molecule of the Year, on December 1991 issue of Science. The Editors made the following observations: Fullerene science exhibits the classic profile of a major scientific breakthrough. Since 1991, the pace of discovery in fullerene science has continued to accelerate. Researchers around the world are exploring both the basics science and potential applications of fullerenes. In 1996, the Nobel Prize in Chemistry was awarded to the codiscoverers, Richard Smalley, Robert Curl and Harry Kroto, for their discovery of fullerenes.

In this paper, we revisit the graph-theoretical formulation of fullerenes and their construction. A fullerene graph is a cubic planar graph with all faces 5-cycles o r6-cycles. Let the number of 5-cycles (pentagons) in a given fullerene F is p and number of 6-cycles (hexagons) is h. Since each vertex lies in exactly 3 faces and each edge lies in 2 faces, then the number of vertices isa v = (5p + 6h)/3, and the number of edges is e = (5p + 6h)/2 = (3/2)v and the number of faces is f = p + h. By the Euler's formula v + e + f = 2, which implies that (5p + 6h)/3 – (5p + 6h)/2 + p + h = 2. Therefore, p =12, v = 2h + 20, e = 3h + 30.

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This paper continues the investigations concerning energy and distance energy of fullerene graphs. Our notation is standard and taken from [13]. We encourage the reader to consult papers [14-32] for background material as well as basic computational techniques.

2. Main results and discussion

In a mechanical system, the stable equilibrium positions minimize the potential energy. The basic geometrical problem of minimizing distance also appears in many contexts. For example, in optics and relativity, light rays follow the paths of minimal distance the geodesics on the curved space-time. In data analysis, the most fundamental method for fitting a function to a set of sampled data points is to minimize the least squares error, which serves as a measurement of the overall deviation between the sample data and the function.

In this section, the eigenvalues of adjacency and distance matrix of many fullerenes are computed. In Table I, we give the energy and distance energy of these fullerenes for $20 \leq p \leq 108$. Then by curve fitting method, we will find a polynomial of the best degree to approximate the energy and distance energy of these fullerenes.

From now on we shall restrict ourselves to a solution given by the theory of asymptotic series and theory of asymptotic expansions. Here the central theme is the construction and investigation of series which represents given functions asymptotically. The functions are often given by integral representations, or by power series, or else appear as solutions of differential equations; and in the latter case the "variable" of the asymptotic expansions may occur either as the independent variable, or else as a parameter, in the differential equation.

Table 1. The Values of E(G) and DE(G) for some Fullerenes

Name	EN	D.EN	No
C_{20}	29.44	100	1
C_{26}	39.71	151.9	2
C_{30}	45.7	202.79	3
C_{40}	61.64	329.44	
C_{48}	74.28	428.69	4
C_{50}	77.4	473.75	5
C_{60}	93.2	642.75	6
C_{70}	108.96	836.15	7
C_{72}	112.04	792.97	8
C_{80}	124.7	1065.3	9
C_{84}	130.66	991.82	10
C_{90}	140.4	1323.2	11
C_{96}	149.92	1204.2	12
C_{108}	168.63	1454.2	13
C_{110}	171.93	1915.7	14
C_{120}	187.5	1738.7	15
C_{144}	225.23	2306.9	16
C_{180}	282.07	3093.7	17

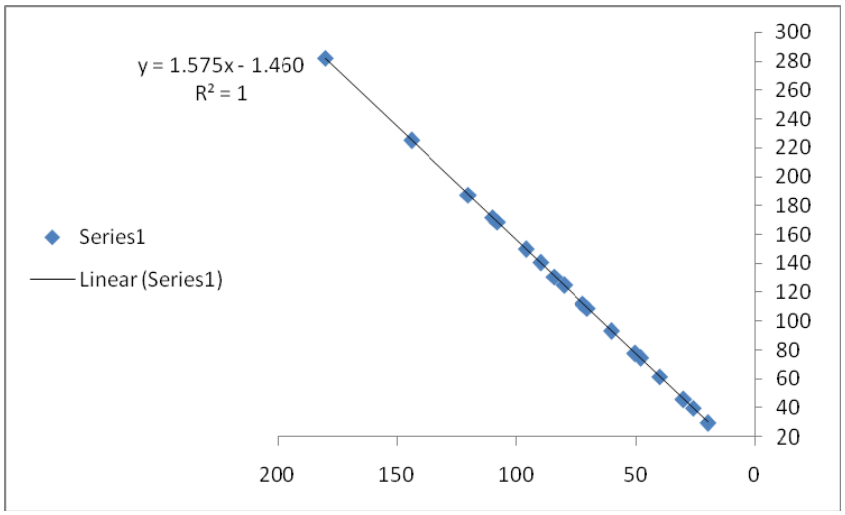

Fig. 1. Energy Regression.

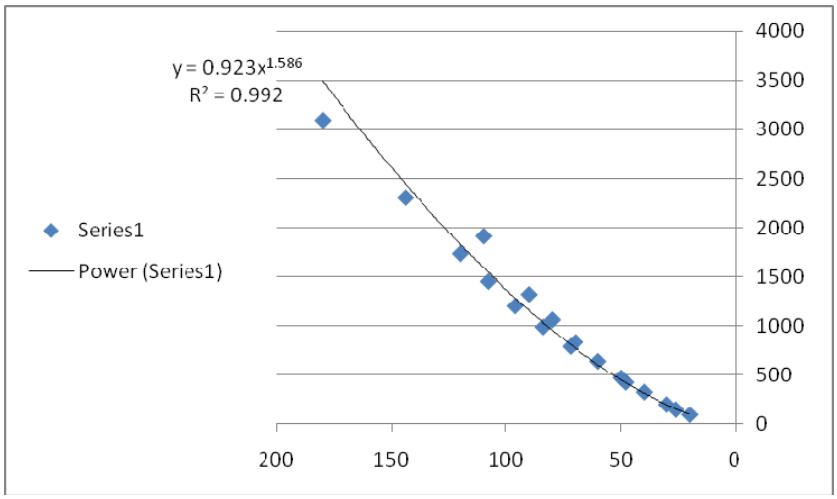

Fig. 2. The Distance Energy Regression.

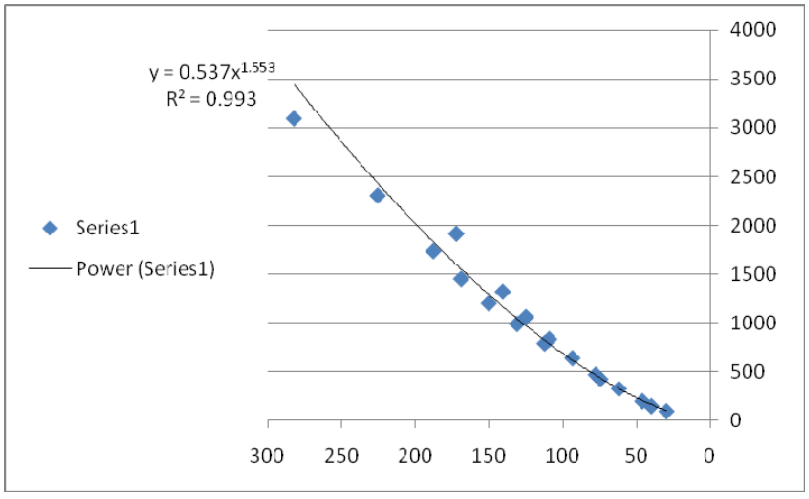

Fig. 3.The power correlation between E(G) and DE(G)

In Figures 1 and 2, diagrams of our calculations are depicted. From these diagrams we conjecture that the energy is tended to a line, asymptotically. But the distance energy probably will be curve. Curve fitting is finding a curve which has the best fit to a series of data points and possibly other constraints. We are interested in curve fitting by power functions, because polynomials are not good for approximating eigenvalues. These figures suggest that the energy and distance energy of these fullerenes and correlation between them can be evaluated by $E(C_n) = 1.575n - 1.460$ $DE(C_n) = .923\, n^{1.586}$ and $DE(C_n) = .537\,(E(C_n))^{1.553}$, respectively.

3. Discussion in behavioral science framework

Establishing different types of correspondences between molecular chemistry and human behavioral sciences is of importance nowadays in the paradigm of multidisciplinary researches. From systems science perspective, we are eagerly looking for unity in the rules and frameworks administrating various aspects of science; either experimental ones, like chemistry or physics, or theoretical ones, like mathematics, or even humanity sciences, like management or human behavior.

One could model the various relationships governing in an organization with fullerene bonds. Fullerene has very tight bindings among its Carbon atoms and constructs a graph, having each vertex 3 neighbors. However one needs to find a correspondence between the energy of every graph or that of its distance matrix with a factor in that organization. Presumably that figures indicate the value of existence or accomplishment of that factor in the organization. Observe that if the value of this factor is linearly proportional to the size of organization or not, is also worth. We are attempting to achieve such types of correspondences between two disciplines in our further researches.

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