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The Second Path Matrix of the Graph and its Characteristic Polynomial

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ABSTRACT. The second path matrix $S(G)$ collects all the second paths in the graph G. Its characteristic polynomial shows some regularity in several particular graphs, such as paths, cycles, stars and complete graphs, as well as in bipartite graphs. Formulas for calculating the characteristic polynomials in these graphs are given. The first eigenvalue of $S(G)$ showed an excellent correlating ability.

1. INTRODUCTION

Let $G = (V, E)$ be a molecular graph with the vertex (atom) set $V = V(G)$ and edge (bond) set E = E(G). $\mathbf{A} = \mathbf{A}(G)$ denotes the n x n *adjacency matrix* of G, which entries are unity if two vertices (atoms) are adjacent and zero otherwise [1,2]. $\mathbf{I} = \mathbf{I}(G)$ stands for the n x n *unit* matrix. In the above, $n = |V(G)|$.

Polynomial description of a molecular graph was used in Quantum Chemistry since the early Hűckel theory, the roots of the most studied *Characteristic Polynomial*:

$$ChA(x, G) = \det[x\mathbf{I} - \mathbf{A}(G)] \qquad (1)$$

being associated to the π-electron energy levels of the molecular orbitals in conjugated hydrocarbons. Other related topics: Topological Resonance Energy TRE, Topological Effect on Molecular Orbitals, TEMO, the Aromatic Sextet Theory, AST, the Kekulé Structure Count, KSC, *etc*.[1-4] make use of the polynomial description of a molecular graph.

Let $a_k = a_k(G)$ denote the coefficients of the characteristic polynomial from the graph G on n vertices:

$$ChA(x, G) = \sum_{k=0}^{n} a_k(G) \cdot x^{n-k} \qquad (2)$$

Formulas for evaluating coefficients a_k make use of either the *Sachs graphs*,[1] contained as subgraphs in G or numeric methods of linear algebra [5,6].

Extension of relation (1) was made by Hosoya [7] and others [8-11] by changing the adjacency matrix with the distance matrix and next by any square topological matrix.

A value y is called an *eigenvalue* of G if and only if $ChA(y,G) = 0$.

A graph G is said to be *bipartite* if each vertex is colored black or white so that adjacent vertices have different colours. In this case the vertex set V(G) is the union of two disjoint sets $B = B(G)$ and $W = W(G)$ of black and white vertices of G, respectively.

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2. SECOND PATH MATRIX

The second path matrix $\mathbf{S} = \mathbf{S}(G)$ is defined as the difference between the squared adjacency matrix and the diagonal matrix $\mathbf{D} = \mathbf{D}(G)$ of vertex degrees in G:

$$\mathbf{S} = \mathbf{S}(G) = \mathbf{A}^2 - \mathbf{D} \tag{3}$$

The characteristic polynomial of S is:

$$ChS(x,G) = \det(x \cdot I - S) = \sum_{k=0}^{n} s_k(G) \cdot x^{n-k} \tag{4}$$

This polynomial is deducible from $ChA(x,G)$ in the case of some simple graphs, such as:

(1) Path: $G = P_n$

$$n = 2k: \qquad ChS(x,P_{2k}) = [ChA(x,P_k)]^2 \tag{5}$$

$$n = 2k+1: \qquad ChS(x,P_{2k+1}) = [ChA(x,P_k)] \cdot [ChA(x,P_{k+1})] \tag{6}$$

(2) Star: $G = S_n$

$$ChS(x,S_n) = x \cdot ChA(x,K_{n-1}) \tag{7}$$

(3) Cycle: $G = C_n$

$$n = 2k: \quad ChS(x,C_{2k}) = [ChA(x,C_k)]^2 \tag{8}$$

$$n = 2k+1: \qquad ChS(x,C_{2k+1}) = ChA(x,C_{2k+1}) \tag{9}$$

(4) Complete graph: $G = K_{n(n>2)}$

$$ChS(x,K_n) = (n-2)^n \cdot ChA\left(\frac{x}{n-2}, K_n\right) \tag{10}$$

$$ChS(x,K_n) = [x-(n-1)(n-2)][x+(n-2)]^{(n-1)} \tag{10'}$$

(5) Complete bipartite graph: $G = K_{w,b}$

$$\begin{aligned} ChS(x,K_{w,b}) &= w^b \cdot b^w \cdot ChA((x-b+w)/b, K_w) \cdot ChA((x-w+b)/w, K_b) \\ &= (x-w(b-1)) \cdot (x-b(w-1) \cdot (x+w)^{(w-1)} \cdot (x+b)^{(b-1)} \end{aligned} \tag{11}$$

(6) Bipartite graph: $G = G(B \cup W, E)$

For a bipartite graph G with $b = |B|$ black vertices and $w = |W|$ white vertices, $b + w = n$, the b x w matrix $\mathbf{C} = \mathbf{C}(G)$ represents the adjacency between the black and white vertices in G. In this case the degree matrix is $\mathbf{D} = (\mathbf{D}_b, \mathbf{D}_w)$ and

$$ChS(x,G) = \det[x \cdot \mathbf{I}_b - (\mathbf{C} \cdot \mathbf{C}^T - \mathbf{D}_b)] \cdot \det[x \cdot \mathbf{I}_w - (\mathbf{C}^T \cdot \mathbf{C} - \mathbf{D}_w)] \qquad (12)$$

$$= [ChA(x,G(B))].[\ ChA(x,G(W))\ ]$$

where $\mathbf{I}_b$ and $\mathbf{I}_w$ denote the b x b and w x w unit matrices, respectively while superscript T refers to the matrix transpose and $G(B)$,$G(W)$ are the two (edge weighted) components corresponding to matrix $\mathbf{S} = \boldsymbol{S}(G)$.
If the bipartite graph $G=G^*$ has the property that $G(B)) = G(W))$, than $ChA(x,G(B)) = ChA(x,G(W))$. For such a (symmetric) graph eq. (12) becomes:

$$ChS(x,G^*) = \{\det[x \cdot \mathbf{I}_b - (\mathbf{C}^2 - \mathbf{D}_b)]\}^2 \qquad (12^*)$$

$$= [ChA(x,G(B))]^2$$

3. EXAMPLES

If $ChS(x,G) = [ChA(s_1(x),G_1)] \cdot [ChA(s_2(x),G_2)]$, graph $G_{1/2}$ have $n_{1/2}$ vertices($n_1 + n_2 = n$), and for i = 1,2,..., n_1, j = 1,2,..., n_2, x_i is an eigenvalue of $\mathbf{A}(G_1)$ then $x_i = s_1(x_{1i})$ ($x_j = s_2(x_{2j})$) and, from this equations, we can calculate the eigenvalue x_{1i} (x_{2j}) of $\mathbf{S}(G)$.

	G	G_1	G_2	x_{1i} and x_{2j}	eq
1	P_5	P_3	P_2	$x_{11} = 2\cos(2\pi \cdot 1/4)$;	6
				$x_{12} = 2\cos(2\pi \cdot 2/4)$;	
				$x_{13} = 2\cos(2\pi \cdot 3/4)$;	
				$x_{21} = 2\cos(2\pi \cdot 1/3)$ and	
				$x_{22} = 2\cos(2\pi \cdot 2/3)$	
2	C_6	C_3	C_3	$x_{11} = 2\cos(2\pi \cdot 1/3)$; $x_{11} = x_{21}$	8
				$x_{12} = 2\cos(2\pi \cdot 2/3)$; $x_{12} = x_{22}$	
				$x_{13} = 2\cos(2\pi)$; $x_{13} = x_{33}$	
3	S_6	K_5	P_1	$x_{11} = 4$, $x_{1i} = -1$ for i=2,3,4,5, and $x_{21} = 0$	7

If $G = C$ is the graph of a cube:

$ChS(x,C) = [2^4 ChA(x/2, T = K_4]^2 = 2^8[ChA(x/2,T)]^2$ and for $x_1 = 3 = s_1(x_{11}) = x_{11}/2$ one obtains $x_{11} = 6 = x_{21}$; for i = 2,3,4 it results $x_i = -1 = s_1(x_{1i}) = x_{1i}/2$ and $x_{1i} = -2 = x_{2i}$.

4. CORRELATING PROPERTIES

The half sum of entries in **S** matrix equals the Gordon-Scantlebury [13] N_2 index.

Platt [14,15] has introduced the total adjacency of edges in a graph, as the *F* index:

$$F = \sum_i \sum_j [\mathbf{EA}]_{ij} = \sum_i \sum_j [\mathbf{S}]_{ij} = 2 \cdot \sum_i \binom{v_i}{2} \tag{13}$$

In eq. (13) $[\mathbf{EA}]_{ij}$ denotes the elements of edge-adjacency matrix. The *F* index is twice the Bertz B_1 index [16], defined as the number of edges in the line graph [17] $L_1(G)$ of *G* and calculated by a combinatorial formula from the vertex valency v_i [18]. Note that **EA** matrix refers to the vertex connectivity in $L_1(G)$.

Despite the summation of all entries in **EA** and **S,** respectively**,** gives the same value [19], (no counter example, so far), the two matrices represent different mathematical objects, leading to different quantities by matrix manipulation. Applications of the above presented topological indices were presented elsewhere [18].

In a recent study, our group [20] found a good correlation of the log*P* in a set of polychlorinated biphenyls (PCBs) with an averaged mass descriptor *AMD* (*i.e*., the mean atomic mass of the vertices at positions 2, 3, and 4 in PCBs, the halogen atom substituent included) and the first eigenvalue *EV* of S, *EV_S*:

$$\log P = -1.790 + 0.654 \cdot AMD + 1.741 \cdot EV\_S \tag{14}$$

$n = 14$; $r = 0.9908$; $s = 0.185$; $CV\% = 2.99$; $F = 296.62$

LOO: $q = 0.984$; Random: $r = 0.583$

A random mixing of the modeled property shows a significant drop in the correlation coefficient value, proving that no chance correlation occurred. The explicit variance is higher than 0.98. Prediction ability of the model (eq 14), as given by "leave-one-out" LOO procedure, is very good ($q = 0.984$). In all, this is an excellent result, even the set of molecules is rather small (see also the result of multivariate regression, reported by the Abraham's group[21]).

5. CONCLUSIONS

The novel matrix **S**, herein proposed, together with its characteristic polynomial, appear as interesting tools in describing the (molecular) graphs. For some particular classes of graphs analytical relations were derived from $ChA(x,G)$. The first eigenvalue of $\mathbf{S}(G)$ showed excellent correlating ability *vs.* log*P* on a set of polychlorinated biphenyls.

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