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Spectral properties of geometric–arithmetic index

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A B S T R A C T

The concept of geometric–arithmetic index was introduced in the chemical graph theory recently, but it has shown to be useful. One of the main aims of algebraic graph theory is to determine how, or whether, properties of graphs are reflected in the algebraic properties of some matrices. The aim of this paper is to study the geometric–arithmetic index GA_1 from an algebraic viewpoint. Since this index is related to the degree of the vertices of the graph, our main tool will be an appropriate matrix that is a modification of the classical adjacency matrix involving the degrees of the vertices. Moreover, using this matrix, we define a GA Laplacian matrix which determines the geometric–arithmetic index of a graph and satisfies properties similar to the ones of the classical Laplacian matrix.

1. Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index, which is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [45]).

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index (R) [34]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [2,15,17,20,25,27,31,36,37,40] and the references therein). During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. The first geometric–arithmetic index GA_1, defined in [44] as

$$GA_1 = GA_1(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u, is one of the successors of the Randić index. Although GA_1 was introduced just a few years ago, there are many papers dealing

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with this index (see, e.g., [9,10,38,39,41,44] and the references therein). There are other geometric–arithmetic indices, like $Z_{p,\,q}$ ($Z_{0,1} = GA_1$), but the results in [9, p. 598] show that the GA_1 index gathers the same information on observed molecule as other $Z_{p,\,q}$ indices.

The reason for introducing a new index is to gain prediction of some property of molecules somewhat better than obtained by already presented indices. Therefore, a test study of predictive power of a new index must be done. The GA_1 index gives better correlation coefficients than Randić index for many physico-chemical properties of octanes, but the differences between them are not significant. However, the predicting ability of the GA_1 index compared with Randić index is reasonably better (see [9, Table 1]). Furthermore, the improvement in prediction with GA_1 index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. Hence, one can think that GA_1 index should be considered in the QSPR/QSAR researches.

Throughout this paper, $G = (V, E) = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) connected graph with $E \neq \emptyset$. Note that the connectivity of G is not an important restriction, since if G has connected components $G_1, \dots, G_r$, then $GA_1(G) = GA_1(G_1) + \cdots + GA_1(G_r)$; furthermore, every molecular graph is connected.

Spectral graph theory is a useful subject that studies the relation between graph properties and the spectrum of some important matrices in graph theory, as the adjacency matrix, the Laplacian matrix, and the incidence matrix, see e.g. [1,6,18]. Eigenvalues of graphs appear in a natural way in mathematics, physics, chemistry and computer science. One of the main aims of algebraic graph theory is to determine how, or whether, properties of graphs are reflected in the algebraic properties of such matrices [18]. Many papers study several topological indices from an algebraic viewpoint (for instance, [21,36,37] study the Randić index, and [39] deals with the geometric–arithmetic index).

The aim of this paper is to obtain new results on the geometric–arithmetic index GA_1 from an algebraic viewpoint. Since this index is related to the degree of the vertices of the graph, our main tool will be an appropriate matrix, denoted by $\mathcal{A}$, that is a modification of the classical adjacency matrix involving the degrees of the vertices. Using $\mathcal{A}$, we will define a GA Laplacian matrix $\mathcal{L}$ and we will prove that it determines the geometric–arithmetic index of a graph; besides, we show that $\mathcal{L}$ satisfies many properties of the classical Laplacian matrix. It is usual to define energies associated to some topological indices (see, e.g., [21]). Along the paper we denote by n the order $n = |V(G)|$ of the graph G and by m its size $m = |E(G)|$. The minimum degree of a graph is denoted by δ and the maximum by Δ. We will denote by $tr(M)$ the trace of the matrix M.

2. Bounds for GA_1

In order to state some bounds for GA_1 we need some previous technical results.

Lemma 2.1. *Let f be the function $f(t) = \frac{2t}{1+t^2}$ on the interval $[0, \infty)$. Then f strictly increases in $[0, 1]$, strictly decreases in $[1, \infty)$, $f(t) = 1$ if and only if $t = 1$ and $f(t) = f(t_0)$ if and only if either $t = t_0$ or $t = t_0^{-1}$.*

Proof. The statements follow from $f'(t) = \frac{2(1-t^2)}{(1+t^2)^2}$. □

Corollary 2.2. *Let g be the function $g(x, y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. Then $\frac{2\sqrt{ab}}{a+b} \le g(x, y) \le 1$. The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$. Besides, $g(x, y) = g(x', y')$ if and only if x/y is equal to either x'/y' or y'/x'. Finally, if $x' < x \le y$, then $g(x', y) < g(x, y)$.*

Proof. It suffices to apply Lemma 2.1, since $g(x, y) = f(t)$ with $t = \sqrt{\frac{x}{y}}$, and $\sqrt{\frac{a}{b}} \le t \le \sqrt{\frac{b}{a}}$. □

We will need the following result.

Proposition 2.3. *Given an $n \times n$ symmetric matrix $B = (b_{ij})$ with $b_{ij} \ge 0$ for every $1 \le i, j \le n$ and the diagonal matrix D with entries $d_{ii} = \sum_{j=1}^n b_{ij}$, then $L := D - B$ is a positive semi-definite matrix.*

Proof. Let $x := (x_1, \dots, x_n) \in \mathbb{R}^n$. Since $x_i^2 + x_j^2 \ge 2x_ix_j$ for every $1 \le i, j \le n$, we have

$$\sum_{i=1}^n \sum_{j=1}^n b_{ij}x_i^2 + \sum_{i=1}^n \sum_{j=1}^n b_{ij}x_j^2 \ge 2\sum_{i=1}^n \sum_{j=1}^n b_{ij}x_ix_j.$$

Since $b_{ij} = b_{ji}$ for every $1 \le i, j \le n$, we conclude

$$xDx^T = \sum_{i=1}^n x_i^2 \sum_{j=1}^n b_{ij} \ge \sum_{i=1}^n \sum_{j=1}^n b_{ij}x_ix_j = xBx^T,$$

and $xLx^T \ge 0$ for every $x \in \mathbb{R}^n$. □