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Research Article

A spectral analysis of the Schultz index

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Abstract: Topological indices are descriptors that assign a number to each molecular graph, often well correlated to some properties. In particular, the Schultz index has stood out for its high discrimination capacity between different molecular structures, being a key tool in the study of their physicochemical properties. In this paper, we introduce a modification of the classical adjacency matrix making use of the Schultz index, incorporating both the degree of the vertices and the distance between each pair of them. We perform a spectral analysis of this index and identify some of its significant properties. Particularly, we focus on determining upper and lower bounds for the eigenvalues of this matrix, contributing to the understanding of its algebraic structure and its relationship with graph parameters.

Keywords: topological indices, Schultz index, matrix of a graph, spectrum of a graph.

AMS Subject classification: 05A05, 05B20, 05C50

1. Introduction

Graph theory has aroused the interest of many researchers due to its wide range of applications in fields such as physics, chemistry, communication sciences, computer technology, engineering, architecture, operational research, genetics, psychology, economics, anthropology, and linguistics, among others. In addition, this discipline has strong connections with fundamental branches of mathematics, such as algebra, matrix theory, numerical analysis, probability, topology, and combinatorics, to

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mention a few. This theory provides a powerful tool for modeling structures and relationships through visual representations of abstract data. Its fundamental elements, vertices and edges, allow to describe interactions and connections between entities. Since its origin in 1736, with Leonhard Euler's famous work on the Königsberg bridge problem [10], this discipline has evolved to become a pillar in the analysis of networks and complex systems. Researchers such as Kirchhoff and Cayley extended its applications to electrical networks [15] and chemical isomers [5], respectively.

Some of its most notable applications are found in chemistry, pharmacology, and biology, through the study of molecular graphs. These graphs represent molecular formulas where the vertices symbolize atoms and the edges the chemical bonds [19]. The physicochemical properties of molecules, essential in these fields, can be correlated with their structure using tools such as topological indices. These indices allow capturing key features of a graph in a single numerical value, which facilitates the analysis of correlations in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) studies [3]. It is known that the first topological index to be introduced was the Wiener index [21], which is defined as the sum of all distances between pairs of vertices of a graph and it allows to model some physical properties such as the boiling point of alkanes. Several indices have been defined since then, such as the MTI proposed by Schultz in 1989 [18], which grants to characterize alkanes and discrimination between different molecular structures. In 1994, Gutman [11] studied this descriptor and defined the Schultz index, also known as distance-degree. This index has been studied from different perspectives, for example, in [9] the authors relate it with that of Wiener for some graph families and in [1] the Schultz index of some graph products is computed explicitly.

One of the most fruitful relationships of graph theory is with matrix theory, in particular, a graph has associated with it various matrices, such as the adjacency matrix, the distance matrix, and the Laplacian matrix, which are essential for computing topological indices. These matrices not only summarize the structure of the graph, but also form the basis of spectral theory of graphs, which analyzes properties of the spectrum associated with these matrices and relates it to parameters of the graph. Although the spectrum does not fully characterize a graph, it provides valuable information about its algebraic and structural properties. Therefore, the fundamental goal of algebraic graph theory is to determine how and to what extent the properties of graphs are reflected in the algebraic properties of certain matrices and vice versa. Spectral graph theory is concerned with investigating the relationship between the eigenvalues of a graph and its structural properties. According to Cvetković [7], this field of study emerged as a result of the work of a considerable number of mathematicians such as L. Collatz, A. J. Hoffman, and H. Sachs. A key paper in this field was the work published in 1957 by Von Collatz and Sinogowitz [20], in which they study finite graphs and their close relationship to non-negative matrix theory.

In recent years, numerous studies have analyzed topological indices from an algebraic perspective, exploring their relationship with matrices associated with graphs.

For example, in [17] the authors studied the geometric-arithmetic index, which depends on the degree of the vertices of the graph. In their study, they introduce a matrix based on the adjacency matrix that incorporates the degrees of the vertices. In addition, they define a geometric-arithmetic Laplacian matrix which presents properties similar to those of the classical Laplacian matrix. On the other hand, in the paper [16] the authors analyze the spectral properties of the inverse sum indeg index, expanding the understanding of the connections between topological indices and algebraic properties of graphs.

This work focuses on the spectral analysis of a matrix associated with a graph that is related to the Schultz index. In particular, a detailed study is carried out to determine upper and lower bounds for the eigenvalues of this matrix, which contributes to the understanding of its algebraic properties and its relationship with the graph structure.

2. Preliminaries

In this section, we state some known results, definitions, and notation used throughout this paper. All graphs considered are finite, undirected, loopless, and without multiple edges. If $\Gamma = (V, E)$ is a graph, its *order* is defined as $|V|$ and its *size* as $|E|$. Two vertices $u, v \in V$ are called *adjacent* if they form an edge, that is, $uv \in E$. By a *walk* from u to v we mean a sequence of vertices

$$u\, x_1\, x_2\, \cdots\, x_k\, v$$

such that any two consecutive are distinct and adjacent, the length of this walk is the number of edges in it, and a *path* from u to v is a walk in which all its vertices are different. Γ is called *connected*, if for every pair of vertices u and v there is a path from u to v. The *distance* between two vertices u and v of a connected graph is defined as

$$d(u, v) = \min\{\text{length}(P) : P \text{ is a path from } u \text{ to } v\}$$

and the *diameter* of Γ is

$$\text{diam}(\Gamma) = \max\{d(u, v) : u, v \in V\}.$$

For a vertex v the *degree* of v is the number of vertices adjacent to it, we denote it by $\deg(v)$, and we denote the maximum and minimum degree of Γ by Δ and δ, respectively.

We know that a graph is completely determined by the adjacency of its vertices and this information can be conveniently organized in matrix form. Given a labeled graph $\Gamma = (V, E)$ of order n, with $V = \{v_1, \ldots, v_n\}$, its *adjacency matrix* is defined as the $n \times n$ matrix $\mathbf{A} = \mathbf{A}(\Gamma)$ over $\mathbb{C}$ with entries

$$\mathbf{A}(i, j) = \begin{cases} 1, & \text{if } v_i v_j \in E; \\ 0, & \text{otherwise.} \end{cases}$$

It can be noted that $\mathbf{A}$ is a symmetric matrix with zero diagonal and the sum of the entries of i-th row is precisely the degree of the vertex v_i. For more concepts and results about graphs see [8, 12].

Now, given a matrix $\mathbf{M} \in \mathrm{Mat}_{n\times n}(\mathbb{C})$, we denote its spectrum by

$$\mathrm{Spec}(\mathbf{M}) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_k \\ m_1 & m_2 & \cdots & m_k \end{pmatrix},$$

and this means that the eigenvalue λ_i has multiplicity m_i, for $i = 1, \ldots, k$.
Recall that the eigenvalues of a real symmetric matrix $\mathbf{M}$ are all real, so they can be ordered $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.
It is known that the *Rayleigh quotients* of a real symmetric matrix $\mathbf{M}$ are key tools for approximating its eigenvalues. For a nonzero vector $\mathbf{Y} \in \mathbb{R}^n$ it is defined as

$$\frac{\mathbf{Y}^t\mathbf{M}\mathbf{Y}}{\mathbf{Y}^t\mathbf{Y}},$$

where $\mathbf{Y}^t$ denotes the transpose of $\mathbf{Y}$. The next result shows the importance of this tool.

Theorem. (Rayleigh Principle) *Let* $\mathbf{M}$ *be a real symmetric* $n \times n$ *matrix with eigenvalues* $\lambda_1 \geq \cdots \geq \lambda_n$*, then* $\lambda_n \leq \mathbf{Y}^t\mathbf{M}\mathbf{Y} \leq \lambda_1$*, for any unitary vector* $\mathbf{Y} \in \mathbb{C}^n$*, with equality in the left-hand (respectively, right-hand) if and only if* $\mathbf{M}\mathbf{Y} = \lambda_n\mathbf{Y}$ *(respectively,* $\mathbf{M}\mathbf{Y} = \lambda_1\mathbf{Y}$*); moreover,*

$$\lambda_1 = \max\left\{\frac{\mathbf{Y}^t\mathbf{M}\mathbf{Y}}{\mathbf{Y}^t\mathbf{Y}} : \mathbf{Y} \neq 0\right\} \quad \textit{and} \quad \lambda_n = \min\left\{\frac{\mathbf{Y}^t\mathbf{M}\mathbf{Y}}{\mathbf{Y}^t\mathbf{Y}} : \mathbf{Y} \neq 0\right\}.$$

The following theorem relates the eigenvalues of a matrix with those of its principal submatrices.

Theorem. (Cauchy) *Let* $\mathbf{M} \in \mathrm{Mat}_{n\times n}(\mathbb{C})$ *be a symmetric matrix with eigenvalues* $\lambda_1 \geq \cdots \geq \lambda_n$ *and let* $\mathbf{B} \in \mathrm{Mat}_{m\times m}(\mathbb{C})$ *be a principal submatrix of* $\mathbf{M}$*, with eigenvalues* $\mu_1 \geq \cdots \geq \mu_m$*, then*

$$\lambda_{n-m+i} \leq \mu_i \leq \lambda_i, \quad \textit{for } i = 1, \ldots, m.$$

Also, recall that a real matrix $\mathbf{M}$ is *non-negative* if all its entries are non-negative, the next result gives a property for the eigenvalues of these matrices.

Theorem. *A non-negative matrix always has a non-negative eigenvalue r such that the moduli of all its eigenvalues do not exceed r. To this maximal eigenvalue an eigenvector with non-negative coordinates corresponds.*

For more concepts and results about matrices, eigenvalues, and topics related see [4, 6, 7, 13, 14].

3. The Schultz matrix of a graph

We start this section by recalling the definition of the Schultz index.

Definition 1. The *Schultz index* of a graph $\Gamma = (V, E)$ is defined by the expression

$$\mathrm{S}(\Gamma) = \frac{1}{2} \sum_{u,v \in V} \big(\deg(u) + \deg(v)\big) d(u, v).$$

It is worth mentioning that some modifications of this index have been made, particularly, in [2], the authors define a generalization as follows

$$\mathrm{S}_{m,n}(\Gamma) = \sum_{u,v \in V} \big(\deg(u) + \deg(v)\big)^m d(u, v)^n.$$

Following the idea of the adjacency matrix of a graph that contains precisely the information of the adjacencies, it can be defined a matrix that encloses the information of the Schultz index.

Definition 2. Let $\Gamma = (V, E)$ be a labeled graph, with $V = \{v_1, \ldots, v_n\}$, the *Schultz matrix* of Γ is defined as the matrix $\mathbf{S} = \mathbf{S}(\Gamma) \in \mathrm{Mat}_{n\times n}(\mathbb{R})$ whose entries are given by

$$\mathbf{S}(i, j) = \big(\deg(v_i) + \deg(v_j)\big) d(v_i, v_j), \quad \text{for } i, j = 1, \ldots, n.$$

We may note that $\mathbf{S}$ has zero diagonal, so that its trace is 0. Moreover, $\mathbf{S}$ is symmetric, thus its eigenvalues are all real. We refer to the spectrum of $\mathbf{S}$ as the *Schultz spectrum* of Γ and we shall write $\mathrm{S\,Spec}(\Gamma)$.

We may observe that the Schultz matrix of a graph depends on the labeling considered to it, but we are interested in those properties that do not depend on it, such as its eigenvalues.

Example 1. Let n be a positive integer and consider the complete graph K_n, which is defined as the graph with vertex set $V = \{v_1, \ldots, v_n\}$ and edge set $E = \{v_iv_j : i \neq j\}$, Figure

1 shows a representation of the complete graph K_8. Since for any two distinct vertices u and v of K_n we have $\deg(u) = \deg(v) = n-1$ and $d(u,v) = 1$, its Schultz matrix is given by

$$\mathbf{S} = \begin{pmatrix} 0 & 2(n-1) & \cdots & 2(n-1) \\ 2(n-1) & 0 & \cdots & 2(n-1) \\ \vdots & & \ddots & \\ 2(n-1) & 2(n-1) & \cdots & 0 \end{pmatrix} = 2(n-1)\begin{pmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & \cdots & 1 \\ \vdots & & \ddots & \\ 1 & 1 & \cdots & 0 \end{pmatrix},$$

but the matrix on the right-hand side is the adjacency matrix $\mathbf{A}$ of K_n. Thus, the eigenvalues of $\mathbf{S}$ are $2(n-1)\lambda$, where λ is an eigenvalue of $\mathbf{A}$. Therefore,

$$\mathrm{S\,Spec}(\mathrm{K}_n) = \begin{pmatrix} 2(n-1)^2 & -2(n-1) \\ 1 & n-1 \end{pmatrix}.$$

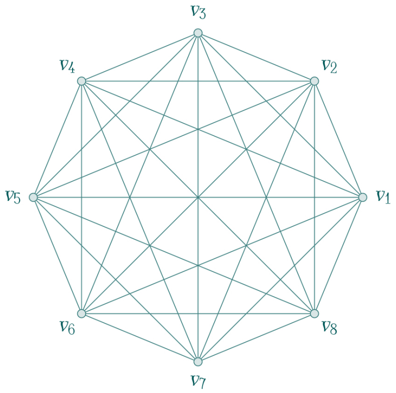

Figure 1. **The complete graph of order 8.**

Observe that if $\mathrm{S}(v_i) = \sum_{j=1}^{n} \big(\deg(v_i) + \deg(v_j)\big) d(v_i, v_j)$, then $\mathrm{S}(v_i)$ is equal to the sum of the entries of the i-th row of $\mathbf{S}$, we denote this expression by S_i, thus,

$$\mathrm{S}(\Gamma) = \frac{S_1 + \cdots + S_n}{2}.$$

Definition 3. Let $\mathbf{S}$ be the Schultz matrix of a labeled graph Γ, we say that Γ is *Schultz-regular*, if $S_1 = \cdots = S_n$.

It can be easily seen that cycle and complete graphs are Schultz-regular.

Lemma 1. *Let $\mathbf{S}$ be the Schultz matrix of a labeled graph Γ, then Γ is Schultz-regular if and only if $\mathbf{Y} = [1 \ \cdots \ 1]^t$ is an eigenvector of $\mathbf{S}$. In fact, $\mathbf{Y}$ is an eigenvector associated to the eigenvalue given by the Schultz-regularity.*

Proof. Assume that Γ is Schultz-regular, then $S_1 = \cdots = S_n = s$, for some $s \in \mathbb{R}$. Observe that

$$\mathbf{SY} = \begin{bmatrix} S_1 \\ \vdots \\ S_n \end{bmatrix} = \begin{bmatrix} s \\ \vdots \\ s \end{bmatrix} = s\mathbf{Y},$$

that is, $\mathbf{Y}$ is an eigenvector of $\mathbf{S}$, with s as the associated eigenvalue.
Now, suppose that $\mathbf{Y}$ is an eigenvector of $\mathbf{S}$, then there exists $s \in \mathbb{R}$ such that $\mathbf{SY} = s\mathbf{Y}$, which implies $S_1 = \cdots = S_n = s$. Therefore, Γ is Schultz-regular. $\square$

Next, we relate the trace of the square of $\mathbf{S}$ with the generalized Schultz index $\mathrm{S}_{2,2}$ of Γ.

Lemma 2. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* $\Gamma = (V, E)$*, then*

$$\operatorname{tr} \mathbf{S}^2 = \mathrm{S}_{2,2}(\Gamma),$$

where $\operatorname{tr} \mathbf{S}^2$ *denotes the trace of* $\mathbf{S}^2$.

Proof. Observe that since $\mathbf{S}$ is symmetric, we have

$$\begin{aligned}
\operatorname{tr} \mathbf{S}^2 &= \mathbf{S}^2(1,1) + \cdots + \mathbf{S}^2(n,n) \\
&= \sum_{j=1}^{n} \mathbf{S}(1,j)\mathbf{S}(j,1) + \cdots + \sum_{j=1}^{n} \mathbf{S}(n,j)\mathbf{S}(j,n) \\
&= \sum_{j=1}^{n} \mathbf{S}(1,j)^2 + \cdots + \sum_{j=1}^{n} \mathbf{S}(n,j)^2 \\
&= \sum_{j=1}^{n} \big(\deg(v_1) + \deg(v_j)\big)^2 d^2(v_1, v_j) + \cdots \\
&\quad + \sum_{j=1}^{n} \big(\deg(v_n) + \deg(v_j)\big)^2 d^2(v_n, v_j) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} \big(\deg(v_i) + \deg(v_j)\big)^2 d^2(v_i, v_j).
\end{aligned}$$

Hence, $\operatorname{tr} \mathbf{S}^2 = \mathrm{S}_{2,2}(\Gamma)$. $\square$

The following result also relates the trace of $\mathbf{S}^2$ but with the Schultz index of Γ, although not with an equality.

Proposition 1. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* $\Gamma = (V, E)$*, then*

$$\frac{\operatorname{tr} \mathbf{S}^2}{4\Delta \operatorname{diam}(\Gamma)} \leq \mathrm{S}(\Gamma) \leq \frac{\operatorname{tr} \mathbf{S}^2}{4\delta}.$$

Proof. Notice that for any $u, v \in V$, the following holds

$$2\delta \leq \big(\deg(u) + \deg(v)\big) d(u, v) \leq 2\Delta \operatorname{diam}(\Gamma).$$

From the proof of the last lemma, we have

$$\operatorname{tr} \mathbf{S}^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \big(\deg(v_i) + \deg(v_j)\big)^2 d^2(v_i, v_j),$$

which implies

$$\begin{aligned} \operatorname{tr} \mathbf{S}^2 &= \sum_{i=1}^{n} \sum_{j=1}^{n} \big(\deg(v_i) + \deg(v_j)\big) d(v_i, v_j) \big(\deg(v_i) + \deg(v_j)\big) d(v_i, v_j) \\ &\leq \sum_{i=1}^{n} \sum_{j=1}^{n} 2\Delta \operatorname{diam}(\Gamma) \big(\deg(v_i) + \deg(v_j)\big) d(v_i, v_j) \\ &= 2\Delta \operatorname{diam}(\Gamma) \sum_{i=1}^{n} \sum_{j=1}^{n} \big(\deg(v_i) + \deg(v_j)\big) d(v_i, v_j), \end{aligned}$$

thus, $\operatorname{tr} \mathbf{S}^2 \leq 4\Delta \operatorname{diam}(\Gamma) \mathrm{S}(\Gamma)$. Analogously, we get the other inequality $\operatorname{tr} \mathbf{S}^2 \geq 4\delta \mathrm{S}(\Gamma)$. □

4. Bounds for the eigenvalues of S

In this section, we propose and prove tight bounds for the eigenvalues of the Schultz matrix of a graph. We start by stating some upper bounds.

Theorem 1. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$*, then*

$$\sigma \leq \sqrt{\frac{(n-1)\mathrm{S}_{2,2}(\Gamma)}{n}}.$$

Moreover, the bound is attained if Γ *is a complete graph.*

Proof. Suppose that $\sigma_1, \sigma_2, \ldots, \sigma_n$ is the complete spectrum of $\mathbf{S}$, with $\sigma = \sigma_1$. Since $\sigma_1 + \sigma_2 + \cdots + \sigma_n = 0$, we have $\sigma_1 = -\sum_{i=2}^{n} \sigma_i$, and by the Cauchy-Schwarz inequality, we get

$$\sigma_1^2 \leq \Big(\sum_{i=2}^{n} 1\Big)\Big(\sum_{i=2}^{n} \sigma_i^2\Big) = (n-1)\sum_{i=2}^{n} \sigma_i^2 = (n-1)\sum_{i=1}^{n} \sigma_i^2 - (n-1)\sigma_1^2,$$

obtaining

$$n\sigma_1^2 \leq (n-1)\sum_{i=1}^{n}\sigma_i^2,$$

but $\sum_{i=1}^{n}\sigma_i^2 = \mathrm{tr}(\mathbf{S}^2) = \mathrm{S}_{2,2}(\Gamma)$, by Lemma 2. Thus,

$$\sigma_1 \leq \sqrt{\frac{(n-1)\mathrm{S}_{2,2}(\Gamma)}{n}}.$$

Now, suppose $\Gamma = \mathrm{K}_n$, then

$$\mathrm{S\,Spec}(\Gamma) = \begin{pmatrix} 2(n-1)^2 & -2(n-1) \\ 1 & n-1 \end{pmatrix},$$

by Lemma 2, we have $\mathrm{S}_{2,2}(\Gamma) = \mathrm{tr}(\mathbf{S}^2)$, but

$$\mathrm{tr}(\mathbf{S}^2) = \sum_{\sigma_i \in \mathrm{S\,Spec\,K}_n} \sigma_i^2 = 4(n-1)^4 + 4(n-1)^3 = 4n(n-1)^3,$$

and since $\sigma = 2(n-1)^2$, this implies

$$(n-1)\mathrm{S}_{2,2}(\Gamma) = 4n(n-1)^4 = n\sigma^2.$$

□

Theorem 2. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$*, then*

$$\sigma \leq 2(n-1)\Delta\,\mathrm{diam}(\Gamma).$$

Moreover, the bound is attained if and only if Γ *is a complete graph.*

Proof. Let $\mathbf{X} = [x_1 \;\cdots\; x_n]^t$ be an eigenvector of $\mathbf{S}$ associated to σ and let $|x_r| = \max\{|x_1|, \cdots, |x_n|\}$. Since $\mathbf{SX} = \sigma\mathbf{X}$, then

$$\begin{aligned} |\sigma x_r| &= \left|\sum_{j=1}^{n}\mathbf{S}(r,j)x_j\right| \leq \sum_{j=1}^{n}\mathbf{S}(r,j)|x_j| \leq \sum_{j\neq r}\mathbf{S}(r,j)|x_r| \\ &\leq |x_r|\sum_{j\neq r}2\Delta\,\mathrm{diam}(\Gamma), \end{aligned}$$

thus, $\sigma \leq 2(n-1)\Delta\,\mathrm{diam}(\Gamma)$.

Now, suppose $\sigma = 2(n-1)\Delta\,\mathrm{diam}(\Gamma)$ and consider an eigenvector $\mathbf{X} = [x_1 \;\cdots\; x_n]^t$ associated to it, such that $x_r = 1$ and $0 \leq x_i \leq 1$, for $i = 1, \ldots, n$. Then

$$2(n-1)\Delta\,\mathrm{diam}(\Gamma) = \sum_{j=1}^{n}\mathbf{S}(r,j)x_j = \sum_{j=1}^{n}\big(\deg(v_r) + \deg(v_j)\big)d(v_r, v_j)x_j,$$

and since $\deg(v) \leq \Delta$ and $d(u,v) \leq \operatorname{diam}(\Gamma)$, for all $u, v \in V$, the above equality implies $\deg(v) = \Delta$, $d(u,v) = \operatorname{diam}(\Gamma) = 1$, and $x_j = 1$, for all $u, v \in V$ and for $j \neq r$. Hence, Γ is a complete graph.
Conversely, if Γ is a complete graph, $\Delta = n-1$, $\operatorname{diam}(\Gamma) = 1$, its largest eigenvalue is $2(n-1)^2$, and the equality holds. ☐

Theorem 3. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$. *If* $s = \max\{S_1, \ldots, S_n\}$, *then* $\sigma \leq s$. *Moreover, the equality holds if and only if* Γ *is Schultz-regular.*

Proof. Since $\mathbf{S} \geq 0$, we can take an eigenvector $\mathbf{X} = [x_1 \ \cdots \ x_n]^t \geq 0$, associated to σ. Let $x_r = \max\{x_1, \ldots, x_n\}$ and observe that $\mathbf{SX} = \sigma\mathbf{X}$ implies

$$\sigma x_r = \sum_{j=1}^{n} \mathbf{S}(r,j)x_j \leq \sum_{j=1}^{n} \mathbf{S}(r,j)x_r \leq s x_r,$$

thus, $\sigma \leq s$.
Now, suppose that Γ is Schultz-regular, by Lemma 1 $\frac{1}{\sqrt{n}}[1 \ \cdots \ 1]^t$ is an eigenvector associated to the eigenvalue s. Thus, Rayleigh's Principle implies $s = \sigma$.
Conversely, assume that s is the largest eigenvalue of $\mathbf{S}$ and consider an eigenvector associated to it $\mathbf{X} \geq 0$. As above, let $x_r = \max\{x_1, \ldots, x_n\}$, then

$$s x_r = \sum_{j=1}^{n} \mathbf{S}(r,j)x_j \leq \sum_{j=1}^{n} \mathbf{S}(r,j)x_r = S_r x_r \leq s x_r,$$

which implies $s = S_r$. So we have

$$s x_r = S_r x_r = \sum_{j=1}^{n} \mathbf{S}(r,j)x_j,$$

obtaining $x_j = x_r$, for $j = 1, \ldots, n$, that is, $[1 \ \cdots \ 1]$ is an eigenvector associated to s. Therefore, by Lemma 1 Γ is Schultz-regular. ☐

Theorem 4. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$. *If* $\bar{S}_i = \sum_{j=1}^{n} \mathbf{S}(i,j)S_j$, *for* $i = 1, \ldots, n$, *and* $\bar{s} = \max\{\bar{S}_1, \ldots, \bar{S}_n\}$, *then*

$$\sigma \leq \sqrt{\bar{s}},$$

and the equality holds if and only if Γ *is Schultz-regular.*

Proof. Let $\mathbf{X} = [x_1 \ \cdots \ x_n]^t$ be a unit eigenvector of $\mathbf{S}$ corresponding to the eigenvalue σ, then

$$\sum_{j=1}^{n} \mathbf{S}(i,j)x_j = \sigma x_i, \quad \text{for } i = 1, \ldots, n,$$

by the Cauchy-Schwarz inequality we get

$$\sigma^2 x_i^2 = \left(\sum_{j=1}^{n} \mathbf{S}(i,j)x_j \right)^2 \leq \sum_{j=1}^{n} \mathbf{S}(i,j) \sum_{j=1}^{n} \left(\sqrt{\mathbf{S}(i,j)} x_j \right)^2 = S_i \sum_{j=1}^{n} \mathbf{S}(i,j)x_j^2,$$

but $\sigma^2 = \sum_{i=1}^{n} \sigma^2 x_i^2$, so we get

$$\begin{aligned} \sigma^2 &\leq \sum_{i=1}^{n} S_i \sum_{j=1}^{n} \mathbf{S}(i,j)x_j^2 = \sum_{j=1}^{n} \left(\sum_{i=1}^{n} \mathbf{S}(i,j) S_i \right) x_j^2 \\ &= \sum_{j=1}^{n} \bar{S}_j x_j^2 \leq \sum_{j=1}^{n} \bar{s} x_j^2 = \bar{s}. \end{aligned}$$

Thus, $\sigma \leq \sqrt{\bar{s}}$.
Now, if $\sigma = \sqrt{\bar{s}}$, we have $\sigma^2 = \bar{s}$ and each of the above inequalities are equalities, particularly,

$$\sum_{i=1}^{n} \sigma^2 x_i^2 = \sum_{i=1}^{n} S_i \sum_{j=1}^{n} \mathbf{S}(i,j)x_j^2,$$

thus,

$$\sum_{i=1}^{n} \left(\sum_{j=1}^{n} \mathbf{S}(i,j)x_j \right)^2 = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} \mathbf{S}(i,j) \sum_{j=1}^{n} \left(\sqrt{\mathbf{S}(i,j)} x_j \right)^2 \right),$$

obtaining

$$\left(\sum_{j=1}^{n} \mathbf{S}(i,j)x_j \right)^2 = \sum_{j=1}^{n} \mathbf{S}(i,j) \sum_{j=1}^{n} \mathbf{S}(i,j)x_j^2, \quad \text{for } i = 1, \ldots, n,$$

which happens if and only if $x_1 = \cdots = x_n$. By Lemma 1, Γ is Schultz-regular.
Conversely, suppose that Γ is Schultz-regular, then $S_1 = \cdots = S_n = s$ is its largest eigenvalue, thus,

$$\bar{S}_i = \sum_{j=1}^{n} \mathbf{S}(i,j)S_j = \sum_{j=1}^{n} \mathbf{S}(i,j)s = s \sum_{j=1}^{n} \mathbf{S}(i,j) = s^2, \quad \text{for } i = 1, \ldots, n,$$

which implies

$$\bar{S}_1 = \cdots = \bar{S}_n = s^2 \quad \text{and} \quad \bar{s} = s^2.$$

Therefore, $\sigma = \sqrt{\bar{s}}$. □

Theorem 5. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$*. If* $\tilde{s}_i = \frac{1}{S_i}\sum_{j=1}^{n} \mathbf{S}(i,j)S_j$*, for* $i = 1, \ldots, n$*, then*

$$\sigma \leq \max\left\{\sqrt{\tilde{s}_i\tilde{s}_j} : 1 \leq i < j \leq n\right\},$$

and the equality holds if and only if Γ *is Schultz-regular.*

Proof. Let $\mathbf{D}$ be the $n \times n$ diagonal matrix whose (i,i) entry is given by S_i, then σ is also the largest eigenvalue of $\mathbf{D}^{-1}\mathbf{S}\mathbf{D}$. Consider an eigenvector $\mathbf{X} = [x_1 \ \cdots \ x_n]^t$ of $\mathbf{S}$ associated to the eigenvalue σ, such that $x_r = 1$ and $x_i \leq 1$, for $i \neq r$, and let $x_t = \max\{x_i : i \neq r\}$. Notice that for $1 \leq i, j \leq n$, we have

$$\mathbf{D}^{-1}\mathbf{S}\mathbf{D}(i,j) = \frac{\mathbf{S}(i,j)S_j}{S_i},$$

then we get

$$\begin{aligned}\sigma x_i = \mathbf{D}^{-1}\mathbf{S}\mathbf{D}\mathbf{X}(i) &= \sum_{j=1}^{n} \mathbf{D}^{-1}\mathbf{S}\mathbf{D}(i,j)\mathbf{X}(j) \\ &= \frac{1}{S_i}\sum_{j=1}^{n} \mathbf{S}(i,j)S_j x_j, \quad \text{for } i = 1, \ldots, n.\end{aligned}$$

In particular, we have

$$\sigma = \frac{1}{S_r}\sum_{j=1}^{n} \mathbf{S}(r,j)S_j x_j \leq \tilde{s}_r x_t \quad \text{and} \quad \sigma x_t = \frac{1}{S_t}\sum_{j=1}^{n} \mathbf{S}(t,j)S_j x_j \leq \tilde{s}_t,$$

thus,

$$\sigma^2 \leq \tilde{s}_r x_t \sigma \leq \tilde{s}_r\tilde{s}_t,$$

that is, $\sigma \leq \sqrt{\tilde{s}_r\tilde{s}_t}$. Hence,

$$\sigma \leq \max\left\{\sqrt{\tilde{s}_i\tilde{s}_j} : 1 \leq i < j \leq n\right\}.$$

Now, suppose that we have the equality $\sigma = \max\left\{\sqrt{\tilde{s}_i\tilde{s}_j} : 1 \leq i < j \leq n\right\}$, then $\sigma = \sqrt{\tilde{s}_r\tilde{s}_t}$ and this implies

$$\tilde{s}_r x_t^2 \leq \tilde{s}_t \quad \text{and} \quad \tilde{s}_t \leq \tilde{s}_r x_t^2,$$

that is, $\tilde{s}_r x_t^2 = \tilde{s}_t$, obtaining $\sigma = \tilde{s}_r x_t$. Thus,

$$\frac{1}{S_r}\sum_{j=1}^{n} \mathbf{S}(r,j)S_j x_j = \frac{1}{S_r}\sum_{j=1}^{n} \mathbf{S}(r,j)S_j x_t,$$

so we get

$$\sum_{j=1}^{n} \mathbf{S}(r,j)\frac{S_j}{S_r}(x_t - x_j) = 0.$$

Now, observe that each summand is non-negative, with $\frac{S_j}{S_r} > 0$, then $x_t - x_j = 0$, for $j \neq r$. Next, note that $\tilde{s}_r x_t^2 = \tilde{s}_t$ implies $\sigma x_t = \tilde{s}_t$, as above, we have

$$\sum_{j=1}^{n} \mathbf{S}(t,j)\frac{S_j}{S_r}(1 - x_j) = 0,$$

and an analogous reasoning shows that $1 - x_j = 0$, for $j \neq t$, obtaining $x_1 = \cdots = x_n = 1$. From this, the sum of the entries of each row of $\mathbf{D}^{-1}\mathbf{SD}$ is constant, that is, $\tilde{s}_1 = \cdots = \tilde{s}_n = \sigma$. Moreover, $\mathbf{D}^{-1}\mathbf{SDX} = \sigma\mathbf{X}$ implies that $\mathbf{DX} = [S_1 \ \cdots \ S_n]^t$ is an eigenvector of $\mathbf{S}$ associated to σ, thus,

$$\sum_{j=1}^{n} \mathbf{S}(i,j) S_j = \sigma S_i, \quad \text{for } i = 1, \ldots, n,$$

but $\sigma = \tilde{s}_1 = \cdots = \tilde{s}_n$, then

$$S_k \sum_{j=1}^{n} \mathbf{S}(i,j) S_j = S_i \sum_{j=1}^{n} \mathbf{S}(k,j) S_j, \quad \text{for } i,k = 1, \ldots, n,$$

and these equalities hold if and only if $S_1 = \cdots = S_n$, that is, if Γ is Schultz-regular. Conversely, if Γ is Schultz-regular, $S_1 = \cdots = S_n = s$ and Theorem 3 implies $\sigma = s$. Observe that

$$s = S_i = \sum_{j=1}^{n} \mathbf{S}(i,j) = \sum_{j=1}^{n} \mathbf{S}(i,j)\frac{s}{s} = \sum_{j=1}^{n} \mathbf{S}(i,j)\frac{S_j}{S_i} = \tilde{s}_i, \quad \text{for } i = 1, \ldots, n,$$

then

$$\sigma = \sqrt{s^2} = \sqrt{\tilde{s}_i \tilde{s}_j}, \quad \text{for } i,j = 1, \ldots, n.$$

Therefore, $\sigma = \max\left\{\sqrt{\tilde{s}_i \tilde{s}_j} : 1 \leq i < j \leq n\right\}$. □

Next, we give some lower bounds for the largest eigenvalue.

Theorem 6. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$*, then*

$$\sigma \geq \frac{2S}{n},$$

where $S = \mathrm{S}(\Gamma)$*, and the equality holds if and only if* Γ *is Schultz-regular.*

Proof. Consider the unit vector $\mathbf{Y} = \frac{1}{\sqrt{n}}\begin{bmatrix}1 & \cdots & 1\end{bmatrix}^t$, then Rayleigh's Principle implies

$$\sigma \geq \frac{\mathbf{Y}^t\mathbf{S}\mathbf{Y}}{\mathbf{Y}^t\mathbf{Y}} = \frac{1}{n}[1 \ \cdots \ 1]\begin{bmatrix}S_1\\ \vdots \\ S_n\end{bmatrix} = \frac{1}{n}\sum_{i=1}^{n} S_i,$$

thus, $\sigma \geq 2S/n$.
Now, let $s = \max\{S_1, \ldots, S_n\}$, since $2S = S_1 + \cdots + S_n$, we have that $2S = ns$ if and only if $S_1 = \cdots = S_n = s$, that is,

$$2S = ns \quad \text{if and only if} \quad \Gamma \text{ is Schultz-regular.}$$

But, by Theorem 3 we know that the last condition is equivalent to σ being s. Thus, Γ is Schultz-regular if and only if $\sigma = 2S/n$. □

Theorem 7. *Let* $\mathbf{S}$ *be the Schultz matrix of a labeled graph* Γ *and let* σ *be the largest eigenvalue of* $\mathbf{S}$*, then*

$$\sigma \geq \sqrt{\frac{S_1^2 + \cdots + S_n^2}{n}},$$

and the equality holds if and only if Γ *is Schultz-regular.*

Proof. Let $\mathbf{X}$ be a unit eigenvector of $\mathbf{S}$ associated to the eigenvalue σ and consider the unit vector $\mathbf{Y} = \frac{1}{\sqrt{n}}[1 \ \cdots \ 1]^t$. If μ is the largest eigenvalue of $\mathbf{S}^2$, then $\sigma^2 = \mu$. Thus,

$$\sigma = \sqrt{\mu} = \sqrt{\mathbf{X}^t\mathbf{S}^2\mathbf{X}} \geq \sqrt{\mathbf{Y}^t\mathbf{S}^2\mathbf{Y}}.$$

On the other hand, observe that

$$\mathbf{Y}^t\mathbf{S}^2\mathbf{Y} = \mathbf{Y}^t\mathbf{S}\mathbf{S}\mathbf{Y} = \mathbf{Y}^t\mathbf{S}^t\mathbf{S}\mathbf{Y} = (\mathbf{S}\mathbf{Y})^t\mathbf{S}\mathbf{Y} = |\mathbf{S}\mathbf{Y}|^2 = \frac{1}{n}\sum_{i=1}^{n} S_i^2,$$

thus, $\sigma \geq \sqrt{\frac{S_1^2+\cdots+S_n^2}{n}}$.
Now, let $s = \max\{S_1, \ldots, S_n\}$ and notice that

$$\sqrt{\frac{S_1^2 + \cdots + S_n^2}{n}} = s \quad \text{if and only if} \quad S_1 = \cdots = S_n = s.$$

Thus, the equality holds if and only if Γ is Schultz-regular. □

Finally, we present a result that gives an upper bound for the least eigenvalue of the Schultz matrix.

Theorem 8. *Let* Γ *be a labeled graph of order* ≥ 2 *and let* $\mathbf{S}$ *be the Schultz matrix of* Γ*. If* σ' *is the least eigenvalue of* $\mathbf{S}$*, then* $\sigma' \leq -2\delta\,\mathrm{diam}(\Gamma)$*. Moreover, the bound is attained if* Γ *is a complete graph.*

Proof. Consider a labeling of Γ such that $d(v_1, v_2)$ realizes the diameter of the graph. Let $\mathbf{M} \in \mathrm{Mat}_{2\times 2}(\mathbb{R})$ be the principal submatrix of $\mathbf{S}$ given by

$$\mathbf{M} = \begin{bmatrix} 0 & \mathbf{S}(1,2) \\ \mathbf{S}(1,2) & 0 \end{bmatrix}$$

and observe that its eigenvalues are $\mu_1 = \mathbf{S}(1,2)$ and $\mu_2 = -\mathbf{S}(1,2)$. If $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ are the eigenvalues of $\mathbf{S}$, Cauchy's theorem implies

$$\sigma_{n-2+2} \leq \mu_2 \leq \sigma_2,$$

that is, $\sigma_n \leq -\mathbf{S}(1,2)$, but

$$\mathbf{S}(1,2) = \big(\deg(v_1) + \deg(v_2)\big)d(v_1, v_2) \geq 2\delta \,\mathrm{diam}(\Gamma),$$

thus, $\sigma' \leq -2\delta$.
Now, if $\Gamma = \mathrm{K}_n$ clearly its least eigenvalue satisfies

$$\sigma' = -2(n-1) = -2\delta(1).$$

□

Conclusions

In this work, we have studied a matrix associated to the Schultz index of a graph obtaining relations between some parameters of this matrix and the Schultz and the generalized Schultz indices. Moreover, our main results are over the largest eigenvalue of the Schultz matrix, getting some bounds for it. After having carried out this study, we consider that we leave the following open problems, among many others.

- Explore possible relations between our results and physical-chemical properties of some molecules.
- Define a Laplacian matrix related to the Schultz index and study it as we did for the Schultz matrix.
- Generalize as much as possible our results for any topological index.

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Data Availability: Data sharing is not applicable to this article as no data sets were generated or analyzed during the current study.

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