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Calculating Szeged Index and Revised Szeged Index by Using Adjacency Matrix

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Abstract
Topological indices are graph invariants used in theoretical chemistry to encode molecules for the design of chemical compounds with given physicochemical properties or given pharmacological and biological activities. Szeged index ($Sz(G)$) and Revised Szeged index ($Sz^*(G)$) of molecular graph identify some distance properties for graphs. In computational chemistry and graph theory, ($Sz(G)$) and ($Sz^*(G)$) were more available to test the characteristics of chemical molecular structures, and thus widely used in chemical applications. In this paper, a simple algorithm is presented for constructing the distance matrix. This algorithm is designed for calculation of $Sz(G)$ and $Sz^*(G)$.

Keywords
Adjacency Matrix; Connected Graph; Distance Matrix; Revised Szeged Index; Szeged Index.

1. INTRODUCTION

Suppose $G = (V, E)$ be a simple and connected graph, with vertex set V and edge set E. Let $n = |V|$ and $m = |E|$ denote the order and the size of G.

The distance between two vertices u and v in graph is the number of edges in the shortest path and is denoted by $d(u, v)$.

Let $e = uv \in E$ and define the partition, with respect to e, $\{N_u(e), N_v(e), N_0(e)\}$ of the vertices of G as follows [1]:

$$N_u(e) = \{w \in V : d(u,w) < d(v,w)\},$$
$$N_v(e) = \{w \in V : d(v,w) < d(u,w)\},$$
$$N_0(e) = \{w \in V : d(v,w) = d(u,w)\}.$$

Let $n_u(e), n_v(e)$ and $n_0(e)$ denote the number of vertices in $N_u(e), N_v(e)$ and $N_0(e)$, respectively. Szeged index [2, 3] of G is defined by

$$Sz = Sz(G) = \sum_{e=uv \in E} n_u(e).n_v(e).$$

The definition of the Szeged index does not take into account the vertices at equal distance to u and v. Szeged star index (or revised Szeged index) of G is defined by [4, 5]:

$$Sz^* = Sz^*(G) = \sum_{e=uv \in E} \left(n_u(e) + \frac{n_0(e)}{2}\right).\left(n_v(e) + \frac{n_0(e)}{2}\right).$$

Some properties and applications of Szeged index and revised Szeged index have been reported in [1, 6, 7, 8, 9, 10].

This paper is organizede in the following way: After introduction, the new algorithm for obtaining $Sz(G)$ and $Sz^*(G)$ is represented in Section 2. In Section 3, effectivness of the proposed approach is verified by solving numerical examples. Finally, conclusions are discussed in the last section.

2. STATEMENT OF THE PROBLEM

The standard distance matrix or the vertex-distance matrix (or the minimum path matrix) of a vertex-labeled connected graph G, denoted by D, is a real symmetrix $n \times n$ matrix whose elements are defined as:

$$D(i,j) = \begin{cases} l(i,j) & if \quad i \neq j, \\ 0 & otherwise, \end{cases}$$

where $l(i,j)$ is the length of the shortest path, i. e., the minimum number of edges, between vertices i and j in G.

This matrix has been used to generate a number of topological indices, e.g., Balaban index [11, 12], Wiener index [13, 14], multiplicative Wiener index [15, 16, 17] and distance-sum index [18]. An efficient algorithm is available for computing the vertex-distance matrix of any graph in [19].

A common way to obtain Matrix D is to use different powers of adjacency Matrix A.

The elements of Matrix A give the connections between vertices. Powers of adjacency matrix are concatenating walks. The $ij-th$ entry of the $k-th$ power of A counts the number of walks of length k from vertex i to vertex j, not paths (a walk can repeat vertices, while a path cannot). So, to

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create a distance matrix, we need to iterativerly power adjacency Matrix A, and as soon as a $ij-th$ element is non-zero, we have to assign the distance k in distance matrix [20].

$A = input('Enetr\ the\ adjacency\ matrix');$
$[n,n] = size(A);$
$D = NaN(n);$
$B = A;$
$k = 1;$
$while\ any(isnan(D(:)))$
$(Check\ for\ new\ walks\ and\ assign\ distance)$
$D(B > 0\ \&\ isnan(D)) = k;$
$(Iteration)$
$k = k + 1;$
$B = B * A;$
$end;$
$(D(i,i) = 2, \quad in\ this\ algorithm)$
$for\ i = 1 : n$
$D(i,i) = 0;$
end

In all the mentioned methods, matrix multiplication is used [19, 20].
In this paper, a simple and practical method for calculating Matrix D, without the need for matrix multiplication will be presented. The advantage of this method is that it can be used for finite graphs with large dimensions and no matrix storage space is necessary.
Matrix D is symmetric with zero diagonal elements. Therefore, in the proposed algorithm, only the elements above diagonal are calculated. Then, the matrix can be obtained by considering symmetry.

Algorithm:
1. Enter adjacency Matrix A,
2. Consider
$$D(i,j) = A(i,j)$$
In this step, all paths with lenght of one are defined.
3. Now starting from $h = 1$ and until all the values above diagonal of Matrix D become non-zero
for $k = 1{:}n$
for $i = k + 1{:}n$
for $j = i + 1{:}n$
if $(A(i,j) = 1 \ \& \ D(k,i) = h \ \& \ D(k,j) = 0)$
$$D(k,j) = h + 1;$$
$$h = h + 1;$$

Thus, for each h, all paths of length $h + 1$ will be specified simultaneously and if all the values above diagonal of Matrix D are non-zero, the algorithm stops.

In [21] theorem 2.2, to calculate $Sz^*(G)$, a formula has been presented based on the number of vertices, the number of edges, N_u, N_v and $Sz(G)$. To use this formula, we need to calculate N_u, N_v and $Sz(G)$. Additionally, in corollary 2.3, for values $Sz(G)$ and $Sz^*(G)$, an upper bound has been identified on the basis of the number of edges and vertices of the graph. In this paper, we will present a simple and applicable algorithm for calculating N_u, N_v, $Sz(G)$ and $Sz^*(G)$ based on distance Matrix D.
Now, with the help of Matrix D and the following algorithm, we can simply calculate $Sz(G)$ and $Sz^*(G)$.
In [8], values $Sz(G)$ and $Sz^*(G)$ for some specific graphs have been achieved based on values of Wiener index. However, for calcilating Wiener index, we need to identify $d(u,v)$ (the number of edges on any of the shortest paths joining vertex u to vertex v) and in this papers, we have presented the method of calculating $d(u,v)$, [8] has not presented a method for calulating it.
Algorithm for calculating $Sz(G)$ and $Sz^*(G)$:
Let

$$Sz = 0, \quad Sz^* = 0, \quad n_i = 0, \quad n_j = 0, \quad n_0 = 0.$$

For all the values above diagonal of Matrix D with $D(i,j) = 1$, (This means that there is an edge e between vertices i and j):
1. for k = 1 : n
calculate $D(i,k) - D(j,k)$,
2. If $D(i,k) - D(j,k) < 0$,
$n_i = n_i + 1$,
(Vertices whose distance from vertex v_j is greater than their distance from vertex v_i)
3. If $D(i,k) - D(j,k) > 0$,
$n_j = n_j + 1$,
4. If $D(i,k) - D(j,k) = 0$,
$n_0 = n_0 + 1$,
We do not need Step 3 to calculate Sz.

$$\begin{cases} Sz^* = Sz^* + \left(n_i + \frac{n_0}{2}\right).\left(n_j + \frac{n_0}{2}\right); \\ Sz = Sz + (n_i).(n_j). \end{cases}$$

3. NUMERICAL EXAMPLES

In this part, some examples are given to study the efficiency of the mentioned method and also to compare it with other solving methods [8].
Example 1: Table (1) shows the values of $Sz(G)$ and $Sz^*(G)$ for some graphs, respectively.
The values obtained for Complete graphs, Complete bipartite graphs and Path graphs are the same as the results found in [8].

The values obtained for Fullerene graphs are the same as those of [22]. Therefore, this algorithm is practical for calculating $Sz(G)$ and $Sz^*(G)$.

Table 1. The values of $Sz(G)$ and $Sz^*(G)$ for special graphs.

G	Sz(G)	$Sz^*(G)$
Complete graphs K_n	$\frac{n(n-1)}{2}$	$\frac{n^3(n-1)}{8}$
K_7	21	257.25
K_8	28	448.00
K_9	36	729.00
Complete bipartite graphs $K_{n,n}$	n^4	n^4
$K_{7,7}$	2401	2401
$K_{8,8}$	4096	4096
$K_{9,9}$	6561	6561
Path graphs P_n	$\frac{n^3-n}{6}$	$\frac{n^3-n}{6}$
P_8	84	84
P_9	120	120
P_{10}	165	165
Fullerene graphs C_n		
C_{72}	95412	139188
C_{84}	163896	222024
C_{96}	235236	331260

Example 2. Let $G = CCC(n)$ be the crystal structure of cubic carbon. values of $Sz(G)$ and $Sz^*(G)$ of $CCC(n)$ for $n = 1$ and $n = 2$ is equal to $Sz(G) = Sz^*(G) = 192$ and $Sz(G) = Sz^*(G) = 4.0704 \times 10^4$. The values obtained for Crystal Structure Cubic Carbon are the same as those of [23].

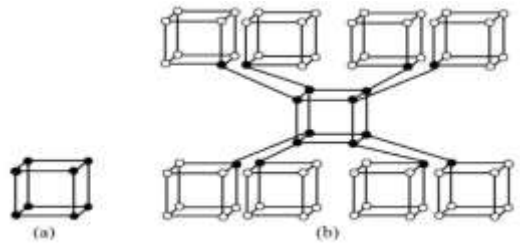

Fig. 1. Crystal Structure Cubic Carbon CCC (1) in part (a) and CCC (2) in part (b).

4. CONCLUSION

Distance Matrix D has been used to generate a number of topological indices. Many studies have been done to find $Sz(G)$ and $Sz^*(G)$ for different graphs. In most cases, the upper and lower bounds are specified for these values. In some graphs, such as Complete graphs and paths, these values are calculated in terms of the number of vertices. In this paper, we calculated D using adjacency matrix and without multiplying the of matrix. Then, using Matrix D, the values of $Sz(G)$ and $Sz^*(G)$ are easily obtained. The results are completely acceptable and satisfactory to compared the mentioned references.

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محاسبه شاخص Szeged و Szeged اصلاح‌شده با استفاده از ماتریس مجاورت

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چکیده

شاخص‌های توپولوژیک مقادیر ثابت مولکولی هستند که در شیمی نظری برای شناسایی طراحی ترکیبات شیمیایی مولکول‌ها با ویژگی‌های فیزیکی شیمیایی داده شده یا فعالیت‌های دارویی و بیولوژیکی معین استفاده می‌شوند. شاخص Szeged (Sz(G)) و Szeged اصلاح‌شده (Sz*(G)) در مولکول، برخی از خصوصیات فاصله را برای نمودارها مشخص می‌کند. در شیمی محاسباتی و نظریه گراف، Sz(G) و Sz*(G) برای تعیین ویژگی‌های ساختارهای مولکولی شیمیایی بیشتر کاربرد دارند و بنابراین به طور گسترده در کاربردهای شیمیایی مورد استفاده قرار می‌گیرند. در این مقاله، یک الگوریتم ساده برای ایجاد ماتریس فاصله ارائه شده است. این الگوریتم برای محاسبه Sz(G) و Sz*(G) استفاده خواهد شد.

واژه‌های کلیدی

ماتریس مجاورت، گراف همبند، ماتریس فاصله، شاخص Szeged اصلاح‌شده، شاخص Szeged.