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Evaluation of Spectral Moments of Signless Laplacian on the Basis of Sub–Graph Contributions and Their Applications to the Zagreb Group Indices

Giorgi Lekishvili

Department of Medicinal Chemistry, Faculty of Pharmacy, Tbilisi State Medical University, 33, Vazha-Pshavela avenue, Tbilisi, Georgia

lekishvili@tsmu.edu

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Abstract

The spectral moments of the signless Laplacian matrix are obtained as function of embedding frequencies of sub-graphs. Higher order spectral moments have been represented also as functions of vertex degrees. We apply these to relate the number of distinct occurrences of sub-graphs with the Zagreb indices.

1. Introduction

The signless Laplacian matrix has found a growing interest among chemical graph theorists. The matrix appears to be a source of powerful topological indices, such as energy-like invariants and Estrada index [1-5]. Clearly, researches of signless Laplacian spectrum are important. In the present paper we extend the use of line graphs to compute the spectral moments of the signless Laplacian matrix for higher orders: It is well known that the signless Laplacian spectrum of a graph G can be determined by the spectrum of the line graph of G. Moreover, by using a result of Estrada [6, 7], we are able to determine these spectral moments as functions of the number of occurrences of sub-graphs, called embedding frequencies. We also give relations of Zagreb group indices with the embedding frequencies of sub-graphs.

The paper is organized as follows: we shall discuss methods, equations and identities required for our study in the first section, next, the main results will be presented and applied to the Zagreb group indices in the third section.

2. Preliminaries

Signless Laplacian matrix **Q** of a simple graph that is undirected and has no multiple edges or loops is given as follows [5]:

$$\mathbf{Q} = \Delta + \mathbf{A} \tag{1.1}$$

Where **Δ** is the diagonal matrix of vertex degrees and **A** is the adjacency matrix. The signless Laplacian relates to the incidence matrix **R** and also to the adjacency matrix ($\mathbf{A}_L$) of the line graph:

$$\mathbf{Q} = \mathbf{R}\mathbf{R}^T \tag{1.2}$$

$$\mathbf{R}^T\mathbf{R} = \mathbf{A}_L + 2\mathbf{I} \tag{1.3}$$

As both $\mathbf{RR}^\mathrm{T}$ and $\mathbf{R}^\mathrm{T}\mathbf{R}$ matrices have the same set of non-zero eigenvalues, one has:

$$\xi_j = \lambda_j + 2 \tag{1.4}$$

Where ξ_k is the j^{th} non-zero eigenvalue of **Q** and λ_k is the j^{th} non-zero eigenvalue of $\mathbf{A}_L$. Therefore, one may express the spectral moments of the signless Laplacian (κ_k) with the help of the spectral moments of the corresponding line graph(μ_k) like the following:

$$\kappa_k = \sum_{i=1}^{n} \xi_i^k = \sum_{j=1}^{m} (2 + \lambda_j)^k \tag{1.5}$$

Where n and m are, correspondingly, the numbers of vertices and of edges.

In the present paper, we are concerned with the first five spectral moments:

$$\kappa_1 = \sum_{j=1}^{m}\left(2 + \lambda_j\right)^1 = 2m + \sum_{j=1}^{m} \lambda_j{}^1 = 2m + \mu_1 \tag{1.6a}$$

$$\kappa_2 = \sum_{j=1}^{m}(2 + \lambda_j)^2 = 4m + 2\sum_{j=1}^{m} \lambda_j{}^1 + \sum_{j=1}^{m} \lambda_j^2 = 4m + 2\mu_1 + \mu_2 \tag{1.6b}$$

$$\kappa_3 = \sum_{j=1}^{m}\left(2 + \lambda_j\right)^3 = \sum_{j=1}^{m}\left(8 + 12\lambda_j + 6\lambda_j^2 + \lambda_j^3\right) = 8m + 12\sum_{j=1}^{m} \lambda_j{}^1 + 6\sum_{j=1}^{m} \lambda_j^2 + \sum_{j=1}^{m} \lambda_j^3 = 8m + 12\mu_1 + 6\mu_2 + \mu_3 \tag{1.6c}$$

$$\kappa_4 = \sum_{j=1}^{m}(2 + \lambda_j)^4 = \sum_{j=1}^{m}(16 + 32\lambda_j + 24\lambda_j^2 + 8\lambda_j^3 + \lambda_j^4) = 16m + 32\sum_{j=1}^{m} \lambda_j{}^1 + 24\sum_{j=1}^{m} \lambda_j^2 + 8\sum_{j=1}^{m} \lambda_j^3 + \sum_{j=1}^{m} \lambda_j^4 = 16m + 32\mu_1 + 24\mu_2 + 8\mu_3 + \mu_4 \tag{1.6d}$$

$$\kappa_5 = \sum_{j=1}^{m}(2 + \lambda_j)^5 = \sum_{j=1}^{m}(32 + 80\lambda_j + 80\lambda_j^2 + 40\lambda_j^3 + 10\lambda_j^4 + \lambda_j^5) = 32m + 80\sum_{j=1}^{m} \lambda_j{}^1 + 80\sum_{j=1}^{m} \lambda_j^2 + 40\sum_{j=1}^{m} \lambda_j^3 + 10\sum_{j=1}^{m} \lambda_j^4 + \sum_{j=1}^{m} \lambda_j^5 = 32m + 80\mu_1 + 80\mu_2 + 40\mu_3 + 10\mu_4 + \mu_5 \tag{1.6e}$$

Estrada gives an expansion of the spectral moments of line graphs via sub-graph contributions [6, 7]:

$$\mu_1 = 0 \tag{1.7a}$$

$$\mu_2 = 2|K_{1,2}| \tag{1.7b}$$

$$\mu_3 = 6\left|K_{1,3}\right| + 6|C_3| \tag{1.7c}$$

$\mu_4 = 2|K_{1,2}| + 12|K_{1,3}| + 24|K_{1,4}| + 4|D_{1,1}| + 12|C_3| + 8|C_4| + 8|C_{3,1}|$ (1.7d)

$\mu_5 = 30|K_{1,3}| + 120|K_{1,4}| + 10|D_{2,1}| + 120|K_{1,5}| + 30|C_3| + 40|C_{3,1}| + 10|\Phi_1| +$
$10|C_{4,1}| + 10|C_5| + 20|C_{3,2}| + 40|\Phi_2|$ (1.7e)

Here, |F| means the embedding frequency (number of distinct occurrences) of a sub-graph F. We use the following notation:

- C_n is a cycle with *n* vertices and K_n is a complete graph with n vertices
- $K_{1,n}$ is a star with one central vertex and *n* pendant vertices
- $D_{k,l}$ is an edge with *k* and *l* pendant vertices attached to its vertices; e.g., $D_{1,1}$ is path-3
- $C_{n,k}$ is a cycle with *n* vertices and *k* pendant vertices attached to one of its vertices
- Φ_1 is a triangle, such that two of its vertices have a pendant vertex (one for each)
- Φ_2 is a quadrangle with a diagonal edge

One has to note that there is a typo in Table 1[7]; it is easy to check that the proper coefficient is 8.

Also, the set of sub-graphs was limited to chemical graphs (i.e., $d_i \leq 4$); we extended the set. The first four spectral moments did not require any amendment, however $K_{1,5}$ stars and $C_{4,1}$(a quadrangle with a pendant vertex attached to one of the vertices of the cycle) had to be considered for the fifth; indeed, each $K_{1,n}$ star produces additional *n*! self-returning walks of length *n* on its line graph, which is K_n, whereas $C_{4,1}$ secures 10 more self-returning walks of length 5; the line graph of $C_{4,1}$ is a pentagon with a diagonal edge.

As is well known, the spectral moments of signless Laplacian can be calculated as functions of vertex degrees [5]. The first three spectral moments can be taken thence (d_i is the degree of the i^{th} vertex):

$\kappa_1 = \sum_{i=1}^{n} d_i = 2m$ (1.8a)

$\kappa_2 = 2m + \sum_{i=1}^{n} d_j^2$ (1.8b)

$\kappa_3 = 6|C_3| + 3\sum_{i=1}^{n} d_j^2 + \sum_{i=1}^{n} d_j^3$ (1.8c)

In order to evaluate the higher order spectral moments of Laplacian, Preciado, Jadbabaie and Verghese employed the Laplacian graph of a simple graph G with *n* edges and *m* vertices [8]. The former is a weighted graph and constructed like the following: it consists of the same set of vertices as G and the set of edges is amended with *n* loops, one for each vertex. The weights on edges were -1; the loops were weighted with vertex degrees, d_i.

The adjacency matrix of the Laplacian graph equals the Laplacian matrix of the corresponding simple graph. Once the k^{th} power of adjacency matrix relates to the number of walks, the k^{th} spectral moment of the Laplacian matrix can be interpreted in terms of the self-returning walks of the length *k*. One may similarly construct the signless Laplacian graph (no weights are applied to edges) and employ the technique designed by Preciado, Jadbabaie and Verghese in appendix of the aforementioned paper [8]. The benefit of the approach is that self-returning walks can be more easily projected onto sub-graphs than semi-edge walks; this might render the use of the former more fruitful than application of the latter.

It must be noted that the method of representation of Laplacian matrices of simple graphs by use of adjacency matrices of the corresponding graphs amended with vertex-degree-weighted loops was first demonstrated by Gutman in 2003 [9]. Moreover, the Laplacian polynomial was explicitly determined as modification of the ordinary characteristic polynomial.

3. Main Results

Application of equations 1.7a-1.7e into equations 1.6a-1.6e results in the following expansions of the signless Laplacian spectral moments as functions of sub-graph contributions:

$$\kappa_1 = 2m \qquad (2.1a)$$

$$\kappa_2 = 4m + 2|K_{1,2}| \qquad (2.1b)$$

$$\kappa_3 = 8m + 12|K_{1,2}| + 6|K_{1,3}| + 6|C_3| \qquad (2.1c)$$

$$\kappa_4 = 16m + 50|K_{1,2}| + 60|K_{1,3}| + 24|K_{1,4}| + 4|D_{1,1}| + 60|C_3| + 8|C_4| + 8|C_{3,1}| \qquad (2.1d)$$

$$\kappa_5 = 32m + 180|K_{1,2}| + 390|K_{1,3}| + 360|K_{1,4}| + 40|D_{1,1}| + 10|D_{2,1}| + 120|K_{1,5}| + 390|C_3| + 80|C_4| + 120|C_{3,1}| + 10|C_{4,1}| + 10|\Phi_1| + 10|C_5| + 20|C_{3,2}| + 40|\Phi_2| \qquad (2.1e)$$

Furthermore, we also calculated the fourth and fifth spectral moments as functions of vertex degrees by employing the technique provided in the appendix of ref 8:

$$\kappa_4 = -\sum_{i=1}^{n} d_i + 2\sum_{i=1}^{n} d_i^2 + 4\sum_{i=1}^{n} d_i^3 + \sum_{i=1}^{n} d_i^4 + 4\sum_{v_i\sim v_j}^{m} d_i d_j + 8\sum_{i=1}^{n} d_i t_i + 8|C_4| \qquad (2.1f)$$

$$\kappa_5 = -5\sum_{i=1}^{n} d_j^2 + 5\sum_{i=1}^{n} d_j^3 + 5\sum_{i=1}^{n} d_j^4 + \sum_{i=1}^{n} d_j^5 - 30|C_3| + 10|C_5| + 10\left(\sum_{v_i\sim v_j}^{m} d_i d_j + \frac{1}{2}\sum_{i=1}^{n}\sum_{j\neq i}^{n} d_i^2 d_j A_{ij} + \sum_{i=1}^{n} d_i t_i + \sum_{i=1}^{n} d_i^2 t_i + \sum_{i=1}^{n} d_i q_i + \sum_{v_i\sim v_j}^{m} N_{ij} d_i d_j\right) \qquad (2.1g)$$

Here, t_i is the number of C_3 sub-graphs (triangles) that are touching (contain) the i^{th} vertex; q_i is the number of C_4 sub-graphs (quadrangles) that are touching (contain) the i^{th} vertex and N_{ij} is the number of common neighbors shared by the i^{th} and j^{th} vertices and A_{ij} is an element of the adjacency matrix.

The equations 2.1a-2.1g present the main result of this contribution.

4. Applications

Equations 2.1f and 2.1g can be rewritten by use of general Zagreb group indices. The first general Zagreb index was introduced by Li and Zheng [10]:

$$M_1^k = \sum_{i=1}^{n} d_i^k \tag{3.1a}$$

The second general Zagreb index was suggested by Xavier, Suresh and Gutman [11]:

$$M_2^k = \sum_{v_i \sim v_j}^{m} \left(d_i d_j\right)^k \tag{3.1b}$$

It is obvious that M_1^2 is the classical M_1 index [12], M_1^3 is the recently re-introduced Forgotten index, F [13] and M_2^1 is the classical M_2.

Therefore, it is plausible to apply equations 2.1f and 2.1g in conjugation with equations 2.1d and 2.1e for elucidation of dependence of vertex-degree-based topological indices on embedding frequencies of sub-graphs.

Let us examine the fourth spectral moment to investigate usefulness of the outlined approach. We shall attempt to reproduce some known identities. A subsequent paper will be dedicated to the fifth spectral moment.

1. First Zagreb Index

A substitution of equation1.8b into equation 2.1b yields:

$$\kappa_2 = 4m + \mu_2 = 4m + 2\left|K_{1,2}\right| = 2m + \sum_{i=1}^{n} d_j^2 \tag{3.2}$$

The first Zagreb group index becomes:

$$M_1 = 2m + 2\left|K_{1,2}\right| \tag{3.2a}$$

(The equation 3.2a seems to be suggested in ref 14, see equation 28 therein.)

2. First General Zagreb Index and F-index

Let us recall that

$$\left|K_{1,2}\right| = 0.5(2m + \sum_{i=1}^{n} d_i^2 - 4m) = 0.5(\sum_{i=1}^{n} d_i^2 - \sum_{i=1}^{n} d_i) = \frac{1}{2}\sum_{i=1}^{n} d_i\,(d_i - 1) \tag{3.3}$$

Now, if we substitute equation3.2a into equation 1.8c and apply it to equation2.1c, we arrive at the following expression:

$$6|C_3| + 3\sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i^3 = 8m + 12\left|K_{1,2}\right| + 6\left|K_{1,3}\right| + 6|C_3| = 6\sum_{i=1}^{n} d_i^2 - 2\sum_{i=1}^{n} d_i + 6\left|K_{1,3}\right| + 6|C_3| \tag{3.4}$$

From equation3.4 we can count the embedding frequency of $K_{1,3}$(the same equation can be derived by use of combinatorial arguments [11, 15]):

$$\left|K_{1,3}\right| = \frac{1}{6}(2\sum_{i=1}^{n} d_i + \sum_{i=1}^{n} d_i^3 - 3\sum_{i=1}^{n} d_i^2) \tag{3.5}$$

The above equation (3.5) can be rewritten as follows:

$$3\sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i^3 = 6\sum_{i=1}^{n} d_i^2 - 2\sum_{i=1}^{n} d_i + 6|K_{1,3}| \qquad (3.6)$$

Therefore,

$$\sum_{i=1}^{n} d_i^3 = 3\sum_{i=1}^{n} d_i^2 - 2\sum_{i=1}^{n} d_i + 6|K_{1,3}| = \sum_{i=1}^{n} d_i^2 + 2(\sum_{i=1}^{n} d_i^2 - \sum_{i=1}^{n} d_i) + 6|K_{1,3}| =$$
$$\sum_{i=1}^{n} d_i^2 + 4|K_{1,2}| + 6|K_{1,3}| = 2m + 6|K_{1,2}| + 6|K_{1,3}| \qquad (3.7)$$

We now see that the F-index can be expressed as follows:

$$F = M_1^3 = \sum_{i=1}^{n} d_i^3 = M_1 + 4|K_{1,2}| + 6|K_{1,3}| \qquad (3.8a)$$

Or

$$F = 2m + 6|K_{1,2}| + 6|K_{1,3}| \qquad (3.8b)$$

The result has been recently reported [11, 15].

As embedding frequencies of any sub-graph are non-negative, from equation 3.5 we also have:

$$3\sum_{i=1}^{n} d_i^2 \le \sum_{i=1}^{n} d_j^3 + 2\sum_{i=1}^{n} d_i \qquad (3.9)$$

Equality holds if and only if the graph in question contains no F_3 sub-graph.

Taking into account that embedding frequencies of $K_{1,4}$ (star with four edges) can also be calculated by use of combinatorial arguments (the same is true for any sub-graph that is a star graph e.g., $|K_{1,3}|$ or $|K_{1,2}|$), we have:

$$|K_{1,4}| = \sum_i \binom{d_i}{4} \qquad (3.10)$$

So that

$$24|K_{1,4}| = \sum_i d_i^4 - 6\sum_i d_i^3 + 11\sum_i d_i^2 - 6\sum_i d_i \qquad (3.11)$$

Now, considering equations 1.8a, 3.2a, 3.7 and 3.11, we immediately arrive at the desirable relationship (reported previously in ref 11):

$$M_1^4 = \sum_i d_i^4 = 2m + 14|K_{1,2}| + 36|K_{1,3}| + 24|K_{1,4}| \qquad (3.12)$$

It is noteworthy that both F-index and M_1^4 depend only on contribution of stars.

3. Second Zagreb Index

Equation 2.1f can be rewritten as follows:

$$\kappa_4 = \sum_{i=1}^{n} d_i + 4\sum_{i=1}^{n} d_i^3 + \sum_{i=1}^{n} d_i^4 + 4\sum_{v_i \sim v_j}^{m} d_i d_j + 8\sum_{i=1}^{n} d_i t_i + 4|K_{1,2}| + 8|C_4| \qquad (3.13)$$

We can apply equation1.8a and equation3.7 to equation3.13:

$$\kappa_4 = 2m + 4(2m + 6|K_{1,2}| + 6|K_{1,3}|) + \sum_{i=1}^{n} d_i^4 + 4\sum_{v_i \sim v_j}^{m} d_i d_j + 8\sum_{i=1}^{n} d_i t_i + 4|K_{1,2}| +$$
$$8|C_4| = 10m + \sum_{i=1}^{n} d_i^4 + 4\sum_{v_i \sim v_j}^{m} d_i d_j + 8\sum_{i=1}^{n} d_i t_i + 28|K_{1,2}| + 24|K_{1,3}| + 8|C_4| \qquad (3.14)$$

Now, we have:

$$4\sum_{v_i \sim v_j}^{m} d_i d_j = \kappa_4 - (10m + \sum_{i=1}^{n} d_i^4 + 8\sum_{i=1}^{n} d_i t_i + 28|K_{1,2}| + 24|K_{1,3}| + 8|C_4|) \qquad (3.15)$$

Application of equation 2.1d into equation3.15 yields:

$4\sum_{v_i\sim v_j}^{m} d_i d_j = 16m + 50|K_{1,2}| + 60|K_{1,3}| + 24|K_{1,4}| + 4|D_{1,1}| + 60|C_3| + 8|C_4| + 8|C_{3,1}| - \left(10m + \sum_{i=1}^{n} d_i^4 + 8\sum_{i=1}^{n} d_i t_i + 28|K_{1,2}| + 24|K_{1,3}| + 8|C_4|\right) = 6m + 22|K_{1,2}| + 36|K_{1,3}| + 24|K_{1,4}| + 4|D_{1,1}| + 60|C_3| + 8|C_{3,1}| - \sum_{i=1}^{n} d_i^4 - 8\sum_{i=1}^{n} d_i t_i$ (3.16)

One may note that M_2does not depend on embedding frequencies of quadrangles as$|C_4|$ is absent in equation 3.16, whichcan be rewritten as follows:

$\sum_{i=1}^{n} d_i^4 + 4\sum_{v_i\sim v_j}^{m} d_i d_j = 6m + 22|K_{1,2}| + 36|K_{1,3}| + 24|K_{1,4}| + 4|D_{1,1}| + 60|C_3| + 8|C_{3,1}| - 8\sum_{i=1}^{n} d_i t_i$ (3.16a)

Eventually, we can express the classicalM_2 index in terms of sub-graph contributions (by substitution of equation 3.12 into equation 3.16a):

$M_2 = \sum_{v_i\sim v_j}^{m} d_i d_j = m + 2|K_{1,2}| + |D_{1,1}| + 15|C_3| + 2|C_{3,1}| - 2\sum_{i=1}^{n} d_i t_i$ (3.17)

It is straightforward to show that

$\sum_{i=1}^{n} d_i t_i = 6|C_3| + |C_{3,1}|$ (3.18)

Therefore, we write:

$$12|C_3| + 2|C_{3,1}| - 2\sum_{i=1}^{n} d_i t_i = 0$$

The aforementioned allows for rewriting equation 3.17 as follows:

$M_2 = m + 2|K_{1,2}| + |D_{1,1}| + 3|C_3|$ (3.19)

Equation 3.19 was reported earlier [11].

By substitution of equation 3.2a into equation 3.19, one also arrives at a lemma that was proved by Vukičević and Pisanski [16] (see also [17, 18]):

$M_2 - M_1 = |D_{1,1}| - m + 3|C_3|$ (3.20)

5. New Topological Index

We shall treat the left-hand sum in equation 3.16a as another (extended) topological index:

$EM_2 = \sum_{i=1}^{n} d_i^4 + 4\sum_{v_i\sim v_j}^{m} d_i d_j = 6m + 22|K_{1,2}| + 36|K_{1,3}| + 24|K_{1,4}| + 4|D_{1,1}| + 12|C_3|$

(3.21)

The modeling and interpretation abilities of the extended index will be researched in subsequent studies.

5. Conclusions

Spectral moments of line graphs have been successfully employed for evaluation of signless Laplacian spectral moments. The latter were also represented as functions of vertex degrees. The main results of the paper will be used for investigations of various topological indices, which are based on the signless Laplacian.

Combined use of the aforementioned representations (functions of sub-graph contributions vs. functions of vertex degrees) suggested a convenient framework for researches of vertex-degree-based topological indices, such as classical and general Zagreb group indices. This approach appears to be quite useful as numerous identities were reproduced with ease; therefore, it can be used for establishing identities, which relate Zagreb group indices with each other [19] and, also, with embedding frequencies of sub-graphs.

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