Iranian J. Math. Chem. 8(1) March (2017) 1−5

Iranian Journal of Mathematical Chemistry

Journal homepage: www.ijmc.kashanu.ac.ir

Stirling Numbers and Generalized Zagreb Indices

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ARTICLE INFO

Article History:

Received 1 January 2016
Accepted 4 March 2016
Published online 5 September 2016
Academic Editor: Sandi Klavžar

Keywords:

Simple graph
Zagreb index
Stirling number

ABSTRACT

We show how generalized Zagreb indices $M_1^k(G)$ can be computed by using a simple graph polynomial and Stirling numbers of the second kind. In that way we explain and clarify the meaning of a triangle of numbers used to establish the same result in an earlier reference.

1. INTRODUCTION AND PRELIMINARIES

The Zagreb indices belong to the oldest and the best researched topological indices.Since their introduction in early seventies [7] they have also given rise to numerous generalizations. (For a survey, see [6].) In this note we show how the information about one of the generalizations, the first general Zagreb index, introduced by Li and Zheng in 2005 [8], can be extracted from a simple, yet neglected, graph polynomial. To the best of our knowledge, the polynomial was introduced and studied in 2008 by two of the present authors and a third one [9], and received no attention afterwards. Crucial to our approach is a family of combinatorial numbers known as the Stirling numbers of the second kind.

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DOI: 10.22052/ijmc.2017.15092

1.1. DEGREE SEQUENCE POLYNOMIAL OF A GRAPH

Let G be a simple connected graph with the degree sequence $\delta = d_1 \le \cdots \le d_m = \Delta$. Its degree sequence polynomial $S_G(x)$ is defined as the generating polynomial of its degree sequence, i.e., as

$$S_G(x) = \sum_{u \in V(G)} x^{d_u} = \sum_{j=\delta}^{\Delta} a_j x^j,$$

where a_j denotes the number of vertices of degree j. The evaluations of the polynomial and its first derivative at 1 give, respectively, the number of vertices and twice the number of edges of G. Hence, $S_G(1) = |V(G)|$ and $S'_G(1) = 2|E(G)|$. Given its simplicity, and proliferation of other graph polynomials, it is surprising that this polynomial attracted no attention of researchers so far. In the following we show that the degree sequence polynomial encodes far more information on G. In order to extract it, we need a family of combinatorial numbers known as Stirling numbers of the second kind.

1.2. STIRLING NUMBERS

The Stirling numbers of the second kind, denoted by $\left\{ n \atop k \right\}$, count the number of partitions of a set of n elements into k non-empty subsets. They form a triangular array whose few beginning rows are shown in Table 1. It can be shown that they satifay a linear recurrence,

$$\left\{ n \atop k \right\} = \left\{ n-1 \atop k \right\} + \left\{ n-1 \atop k-1 \right\}$$

for $n > 0$ with the initial conditions $\left\{ 0 \atop 0 \right\} = 1$ and $\left\{ 0 \atop j \right\} = \left\{ 0 \atop i \right\} = 0$ for all $i, j \neq 0$. We refer the reader to [5] for a thorough discussion of these numbers and their properties. The most important for us is the fact that the Stirling numbers of the second kind are used to convert between powers and falling factorials,

$$x^n = \sum_k \left\{ n \atop k \right\} x^{\underline{k}},$$

where $x^{\underline{k}}$ is the falling factorial defined as $x^{\underline{k}} = x(x-1)\ldots(x-k+1)$. The opposite relationship,

$$x^{\underline{n}} = \sum_k \left[n \atop k \right] (-1)^{n-k} x^k,$$

involves the Stirling numbers of the first kind $\begin{bmatrix} n \\ k \end{bmatrix}$ that count the ways to arrange n objects into cycles. In the rest of the paper we will make use of both conversion formulas.

Table 1. Stirling numbers of the second kind $\left\{ \begin{matrix} n \\ k \end{matrix} \right\}$.

n/k	0	1	2	3	4	5	6
0	1						
1	0	1					
2	0	1	1				
3	0	1	3	1			
4	0	1	7	6	1		
5	0	1	15	25	10	1	
6	0	1	31	90	65	15	1

1.3. GENERALIZED ZAGREB INDICES

Recall that the first and the second Zagreb indices are defined as

$$M_1(G) = \sum_{u \in V(G)} d_u^2 \qquad and \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

respectively, where d_u denotes the degree of vertex u. The k-th general first Zagreb index $M_1^k(G)$ is defined [8] as the sum of k-th powers of degrees of vertices of G, $M_1^k(G) = \sum_{u \in V(G)} d_u^k$. Hence, $M_1^1(G) = 2|E(G)|$ and $M_1^2(G) = M_1(G)$. For $k = 3$ one obtains the forgotten index $F(G)$ [4]. Our main result shows that all information about $M_1^k(G)$ for all k is encoded in the degree sequence polynomial of G.

2. MAIN RESULTS

Theorem 1. Let G be a simple connected graph and $S_G(x)$ its degree sequence polynomial. Then the k–th general Zagreb index of G can be computed as

$$M_1^k(G) = \sum_{j=1}^{k} \left\{ \begin{matrix} k \\ j \end{matrix} \right\} S_G^{(j)}(1)$$

for any $k \in \mathbb{N}$.

Proof.

$$M_1^k(G) = \sum_{u\in V(G)} d_u^k = \sum_{u\in V(G)} \sum_j \left\{ {k \atop j} \right\} d_u^j = \sum_j \left\{ {k \atop j} \right\} \sum_{u\in V(G)} d_u^j = \sum_j \left\{ {k \atop j} \right\} S_G^{(j)}(1).$$

Corollary 2.

$$S_G^{(k)}(1) = \sum \left[{k \atop j} \right] (-1)^{k-j} M_1^j(G).$$

As an example, we look at the case of tetrameric 1,3–adamantane, considered by Fath–Tabar *et al.* in reference [3]. It is clear by inspection that a chain $TA[n]$ of n such units has $6n$ vertices of degree 2, $2n+2$ vertices of degree 3 and $2n-2$ vertices of degree 4. Hence, its degree sequence polynomial is given by $S_{TA[n]} = 6nx^2 + 2(n+1)x^3 + 2(n-1)x^4$. From there, by using Theorem 1, we immediately obtain $M_1^2(TA[n]) = M_1(TA[n]) = 74n-14$ (as obtained in [3]), $M_1^3(TA[n]) = 230n-74$ and $M_1^4(TA[n]) = 770n-350$.

3. CONCLUDING REMARKS

The same approach we used here could be applied to other topological indices and polynomials. For example, there are variants of eccentricity polynomials that encode the information about sums of powers of vertex eccentricities [2].

A comparable approach to degree–based topological indices was employed by Deutsch and Klavžar [1]. Their M–polynomial is a bivariate generating polynomial encoding the information about the number of edges whose end–vertices have certain degrees. It allows quick finding of any degree–based graph invariant, but it takes more work to compute the polynomial than in the case of degree sequence polynomial.

We conclude by mentioning that our results were anticipated in some earlier papers, but the relationship was never made explicit. For example, in Theorem 3.1 of reference [10] concerned with general Zagreb indices, $M_1^k(G)$ are given as sums of the numbers of (not necessarily induced) star subgraphs of G multiplied by certain coefficients. The coefficients form a triangular array $t_{n,k}$ and it can be easily guessed that $t_{n,k} = k!\left\{ {n \atop k} \right\}$. Our results provide an elegant proof. Similar observation can be made about the triangle of coefficients in Corollary 3.1 of the same reference.

ACKNOWLEDGMENT. Partial support of the Croatian Science Foundation under the project 8481 (BioAmpMode) is gratefully acknowledged by the first author. We are thankful to the anonymous referee for careful reading and useful suggestions.

REFERENCES

1. E. Deutsch, S. Klavžar, *M*–polynomial and degree–based topological indices, *Iranian J. Math. Chem.* **6** (2015) 93–102.
2. T. Došlić, M. Ghorbani, M. A. Hosseinzadeh, Eccentric connectivity polynomial of some graph operations, *Util. Math.* **84** (2011) 297–309.
3. G. H. Fath–Tabar, A. Azad, N. Elahinezhad, Some topological indices of tetrameric 1,3–adamantane, *Iranian J. Math. Chem.* **1** (2010) 111–118.
4. B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.
5. R. L. Graham, D. E. Knuth, O. Patashnik, *Concrete Mathematics*, Addison–Wesley, Reading, 1988.
6. I. Gutman, K. Ch. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
7. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
8. X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.
9. S. Sedghi, N. Shobe, M. A. Salahshoor, The polynomials of a graph, *Iranian J. Math. Sci. Inf.* **3** (2008) 55–68.
10. G. B. A. Xavier, E. Suresh, I. Gutman, Counting relations for general Zagreb indices, *Kragujevac J. Math.* **38** (2014) 95–103.