昆明学院学报　2019，41（3）：69～73　ISSN 1674－5639　CN 53－1211/G4
Journal of Kunming University

循环图的萨格勒布多项式和重新定义的萨格勒布指数

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摘要：拓扑指数是与图相关联的数值，其有助于预测潜在图形的诸多属性．循环图由于其特殊的结构，可表示诸多化合物的分子构造，因而在分子图的建模中常被视为基本结构之一，并嵌入到其他分子结构中．因此，利用图结构分析、边划分和代数方法，计算循环图的萨格勒布多项式．此外，计算了重新定义的循环图的萨格勒布指数．

关键词：萨格勒布指数；Randic 指数；多项式；度；图
中图分类号：O157.6　**文献标识码**：A　**文章编号**：1674－5639（2019）03－0069－05
DOI：10.14091/j.cnki.kmxyxb.2019.03.015

Zagreb Polynomials and Redefined Zagreb Indices of Circulant Graph

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Abstract：Topological indices are numerical numbers associated with a graph that helps to predict many properties of underlined graph. Due to its special structure, the circulant graph represents the molecular structure of many compounds. Therefore, it is often regarded as one of the basic structures in the modeling of molecular graphs and embedded in other molecular structures. In this paper, by means of graph structure analysis, edge dividing and algebraic tricks, we aim to compute Zagreb polynomials of circulant graph and redefined Zagreb indices of circulant graph.

Key words：Zagreb index；Randic index；polynomial；degree；graph

0　Introduction

A number, polynomial or a matrix can uniquely identify a graph. A topological index is a numeric number associated to a graph which completely describes the topology of the graph, and this quantity is invariant under the isomorphism of graphs. The degree-based topological indices are derived from degrees of vertices in the graph. These indices have many correlations to chemical properties. In other words, a topological index remains invariant under graph isomorphism. The study of topological indices, based on distance in a graph, was effectively introduced in 1947 in chemistry by Weiner[1]. He introduced a distance-based topological index called the "Wiener index" to correlate properties of alkenes and the structures of their molecular graphs. Recent progress in nano-technology is attracting attention to the topological indices of molecular graphs, such as nanotubes, nanocones, and fullerenes to cut short experimental labor. Since their introduction, more than 140 topological indices have been developed, and experiments reveal that these indices, in combination, determine the material properties such as melting point, boiling point, heat of formation, toxicity, toughness, and stability[2]. These indices play a vital role in computational and theoretical aspects of chemistry in predicting material properties[3].

Several algebraic polynomials have useful applications in chemistry, such as the Hosoya Polynomial (also

收稿日期：2019－03－09
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called the Wiener polynomial)[4]. It plays a vital role in determining distance-based topological indices. Among other algebraic polynomials, the M polynomial introduced recently in 2015[5] plays the same role in determining the closed form of many degree-based topological indices. Other famous polynomials are the first Zagreb polynomial and the second Zagreb polynomial.

A graph G is an ordered pair (V, E), where V and E vertices and edges of G respectively. A graph is connectedif there is a path between every pair of vertices in it. Graph theory is contributing a lion's share in many areas such as chemistry, physics, pharmacy, as well as in industry[6]. We will start with some preliminary facts.

The first and the second Zagreb indices are defined as:

$$M_1(G)=\sum_{uv\in E(G)}(d_u+d_v),$$

and

$$M_2(G)=\sum_{uv\in E(G)}(d_u\times d_v).$$

For details see[7]. Considering the Zagreb indices, Fath-Tabar[8] defined first and the second Zagreb polynomials as:

$$M_1(G,x)=\sum_{uv\in E(G)}x^{d_u+d_v},$$

and

$$M_2(G,x)=\sum_{uv\in E(G)}x^{d_u\times d_v}.$$

The properties of $M_1(G,x)$, $M_2(G,x)$ polynomials for some chemical structures have been studied in the literature[7].

After that, in [9], the authors defined the third Zagreb index

$$M_3(G)=\sum_{uv\in E(G)}(d_u-d_v),$$

and the polynomial

$$M_3(G,x)=\sum_{uv\in E(G)}x^{d_u-d_v}.$$

In the year 2016[10], following Zagreb type polynomials were defined

$$M_4(G,x)=\sum_{uv\in E(G)}x^{d_u(d_u+d_v)};$$

$$M_5(G,x)=\sum_{uv\in E(G)}x^{d_v(d_u+d_v)};$$

$$M_{a,b}(G,x)=\sum_{uv\in E(G)}x^{ad_u+bd_v};$$

$$M'_{a,b}(G,x)=\sum_{uv\in E(G)}x^{(d_u+a)(d_v+b)}.$$

Ranjini et al.[11] redefined the Zagreb index, i. e., the redefined first, second and third Zagreb indices of graph G. These indicators appear as:

$$\mathrm{Re}ZG_1(G)=\sum_{uv\in E(PD_1)}\frac{d_u+d_v}{d_u\times d_v};$$

$$\mathrm{Re}ZG_2(G)=\sum_{uv\in E(PD_1)}\frac{d_u\times d_v}{d_u+d_v};$$

$$\mathrm{Re}ZG_3(G)=\sum_{uv\in E(PD_1)}(d_u\times d_v)(d_u+d_v).$$

In this paper we compute other Zagreb polynomials and Redefined Zagreb indices of circulant graphs. For details about applications of graph theory, please see [12—16] and references therein.

Definition 1 Let n, m, and a_1, a_2, $\cdots$, a_m be positive integers, where $1\leqslant a_i\leqslant[n/2]$ and $a_i\neq a_j$ for all $1\leqslant i<j\leqslant m$. An undirected graph with the set of vertices $V=\{v_1,v_2,\cdots,v_n\}$ and the set of edges $E=\{v_iv_{i+a_i}: 1\leqslant i\leqslant n,\ 1\leqslant j\leqslant m\}$ where the indices being taken modulo in n, is called the circulant graph, and is denoted by $C_n(a_1,a_2,\cdots,a_m)$.

The graph of $C_{10}(2,3)$ is shown in Figure 1.

This is one of the most comprehensive families, as its specializations give some important families. Classes of graphs that are circulant include the Andrásfai graphs, antiprism graphs, cocktail party graphs, complete graphs, complete bipartite graphs, crown graphs, empty graphs, rook graphs, Möbius ladders, Paley graphs of prime order, prism graphs, and torus grid graphs.

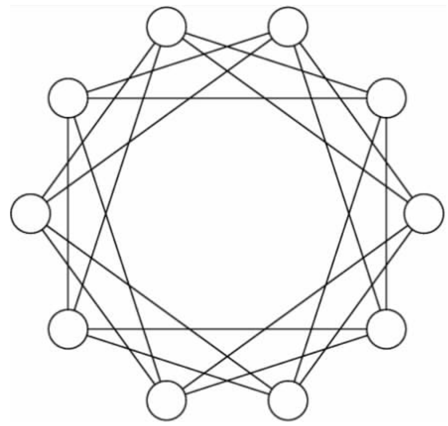

Figure 1 $C_{10}(2,3)$

1 Computational Results

Theorem 1 Let $C_n(a_1,a_2,\cdots,a_m)$ be a Circulant graph. Then

1) $M_3(C_n(a_1,a_2,\cdots,a_m),x)=n$;

2) $M_4(C_n(a_1,a_2,\cdots,a_m),x)=nx^{2(n-1)^2}$;

3) $M_5(C_n(a_1,a_2,\cdots,a_m),x)=nx^{2(n-1)^2}$;

4) $M_{a,b}(C_n(a_1,a_2,\cdots,a_m),x)=nx^{(n-1)(a+b)}$;

5) $M'_{a,b}(C_n(a_1,a_2,\cdots,a_m),x)=nx^{(n-1+a)(n-1+b)}$.

Proof Let $C_n(a_1,a_2,\cdots,a_m)$ be the Circulant graph, where $n=3, 4, \cdots, n$ and $1\leqslant a_i\leqslant [n/2]$ and $a_i\neq a_j$ when n is even and $1\leqslant a_i\leqslant [n/2]$, $a_i\leqslant a_j$ when n is odd. It is clear from the graph of $C_n(a_1,a_2,\cdots,a_m)$ that circulant graph only has one partition of vertex set i. e.,

$$V_1=\{v\in V(C_n(a_1,a_2,\cdots,a_m))\mid d_v=n\}.$$

The edge set of $C_n(a_1,a_2,\cdots,a_m)$ has the following one partition,

$$E_1=E_{\{n-1,n-1\}}=\{e=uv\in E(C_n(a_1,a_2,\cdots,a_m))\mid d_u=d_v=n-1\},$$

Now

$$|E_1(C_n(a_1,a_2,\cdots,a_m))|=n.$$

1) $$M_3((C_n(a_1,a_2,\cdots,a_m)),x)=\sum_{uv\in E(C_n(a_1,a_2,\cdots,a_m))}x^{d_v-d_v}=\sum_{uv\in E_1(C_n(a_1,a_2,\cdots,a_m))}x^{(n-1)-(n-1)}=n.$$

2) $$M_4((C_n(a_1,a_2,\cdots,a_m)),x)=\sum_{uv\in E(C_n(a_1,a_2,\cdots,a_m))}x^{d_u(d_u+d_v)}=\sum_{uv\in E_1(C_n(a_1,a_2,\cdots,a_m))}x^{(n-1)[(n-1)+(n-1)]}=|E_1(C_n(a_1,a_2,\cdots,a_m))|x^{2(n-1)^2}=nx^{2(n-1)^2}.$$

3) $$M_5((C_n(a_1,a_2,\cdots,a_m)),x)=\sum_{uv\in E(C_n(a_1,a_2,\cdots,a_m))}x^{d_v(d_u+d_v)}=\sum_{uv\in E_1(C_n(a_1,a_2,\cdots,a_m))}x^{(n-1)[(n-1)+(n-1)]}=|E_1(C_n(a_1,a_2,\cdots,a_m))|x^{2(n-1)^2}=nx^{2(n-1)^2}.$$

4) $$M_{a,b}((C_n(a_1,a_2,\cdots,a_m)),x)=\sum_{uv\in E(C_n(a_1,a_2,\cdots,a_m))}x^{(ad_u+bd_v)}=\sum_{uv\in E_1(C_n(a_1,a_2,\cdots,a_m))}x^{[(n-1)a+(n-1)b]}=|E_1(C_n(a_1,a_2,\cdots,a_m))|x^{(n-1)(a+b)}=nx^{(n-1)(a+b)}.$$

5) $$M'_{a,b}((C_n(a_1,a_2,\cdots,a_m)),x)=\sum_{uv\in E(C_n(a_1,a_2,\cdots,a_m))}x^{(d_u+a)(d_v+b)}$$

$$= \sum_{uv \in E_1(C_n(a_1,a_2,\cdots,a_m))} x^{(n-1+a)(n-1+b)}$$
$$= |E_1(C_n(a_1,a_2,\cdots,a_m))| x^{(n-1+a)(n-1+b)}$$
$$= nx^{(n-1+a)(n-1+b)}.$$

Theorem 2 Let $C_n(a_1,a_2,\cdots,a_m)$ be the Circulant graph. Then,

1) $ReZG_1(C_n(a_1,a_2,\cdots,a_m)) = \frac{2n}{n-1}$;

2) $ReZG_2(C_n(a_1,a_2,\cdots,a_m)) = \frac{n(n-1)}{2}$;

3) $ReZG_3(C_n(a_1,a_2,\cdots,a_m)) = 2n(n-1)^3$.

Proof

1) $$ReZG_1(C_n(a_1,a_2,\cdots,a_m)) = \sum_{uv \in E(C_n(a_1,a_2,\cdots,a_m))} \frac{d_u + d_v}{d_u \times d_v}$$
$$= \sum_{uv \in E_1(C_n(a_1,a_2,\cdots,a_m))} \frac{(n-1)+(n-1)}{(n-1)\times(n-1)}$$
$$= |E_1(C_n(a_1,a_2,\cdots,a_m))| \frac{2(n-1)}{(n-1)^2}$$
$$= \frac{2n}{n-1}.$$

2) $$ReZG_2(C_n(a_1,a_2,\cdots,a_m)) = \sum_{uv \in E(C_n(a_1,a_2,\cdots,a_m))} \frac{d_u \times d_v}{d_u + d_v}$$
$$= \sum_{uv \in E_1(C_n(a_1,a_2,\cdots,a_m))} \frac{(n-1)\times(n-1)}{(n-1)+(n-1)}$$
$$= |E_1(C_n(a_1,a_2,\cdots,a_m))| \frac{(n-1)^2}{2(n-1)}$$
$$= \frac{n(n-1)}{2}.$$

3) $$ReZG_3(C_n(a_1,a_2,\cdots,a_m)) = \sum_{uv \in E(C_n(a_1,a_2,\cdots,a_m))} (d_u \times d_v)(d_u + d_v)$$
$$= \sum_{uv \in E_1(C_n(a_1,a_2,\cdots,a_m))} ((n-1)\times(n-1))((n-1)+(n-1))$$
$$= 2(n-1)^3 |E_1(C_n(a_1,a_2,\cdots,a_m))|$$
$$= 2n(n-1)^3.$$

2 Conclusion

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index, known as a connectivity index, is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. In this paper, we computed Zagreb polynomials and redefined Zagreb indices of Circulant graphs.

[References]

[1] WIENER H. Structural determination of paraffin boiling points [J]. Journal of the American Chemical Society, 1947, 69: 17 -20.

[2] KATRITZKY A R, JAIN R, LOMAKA A, et al. Perspective on the relationship between melting points and chemical structure [J]. Crystal Growth Design, 2001 (1): 261 -265.

[3] RUCKER G, RUCKER C. On topological indices, boiling points, and cycloalkanes [J]. Journal of Chemical Information and Computer Sciences, 1999, 39: 788 - 802.

[4] GUTMAN I. Some properties of the wiener polynomial [J]. Graph Theory Notes, 1993, 125: 13 - 18.

[5] KLAVZAR S, DEUTSCH E. M-polynomial and degree-based topological indices [J]. Iranian Journal of Mathematical Chemistry, 2015, 6: 93 - 102.

[6] GUTMAN I, TRINAJSTIC N. Graph theory and molecular orbitals total pi-electron energy of alternant hydrocarbons [J]. Chemical Physics Letters, 1972, 17: 535 - 538.

[7] GUTMAN I, DAS K C. The first Zagreb index 30 years after [J]. MATCH Communications in Mathematical and in Computer Chemistry, 2004, 50: 83 - 92.

[8] FATH-TABAR G H. Old and new Zagreb index [J]. MATCH Communications in Mathematical and in Computer Chemistry, 2011, 65: 79 - 84.

[9] FATH-TABAR G H. Zagreb polynomial and pi indices of some nano structures [J]. Digest Journal of Nanomaterials and Biostructures, 2009, 4 (1): 189 - 191.

[10] BINDUSREE A R, CANGUL I N, LOKESHA V, et al. Zagreb polynomials of three graph operators [J]. Filomat, 2016, 30 (7): 1979 - 1986.

[11] RANJINI P S, LOKESHA V, USHA A. Relation between phenylene and hexagonal squeeze using harmonic index [J]. Intentional Journal of Graph Theory, 2013 (1): 116 - 121.

[12] TANG Z H, LIANG L, GAO W. Wiener polarity index of quasi-tree molecular structures [J]. Open Journal of Mathematical Sciences, 2018, 2 (1): 73 - 83.

[13] LIU G S, JIA Z Y, GAO W. Ontology similarity computing based on stochastic primal dual coordinate technique [J]. Open Journal of Mathematical Sciences, 2018, 2 (1): 221 - 227.

[14] SARDAR M S, PAN X F, GAO W, et al. Computing sanskruti index of titania nanotubes [J]. Open Journal of Mathematical Sciences, 2017, 1 (1): 126 - 131.

[15] GAO W, MUZAFFAR B, NAZEER W. K-banhatti and k-hyper banhatti indices of dominating david derived network [J]. Open Journal of Mathematical Sciences, 2017, 1 (1): 13 - 24.

[16] GAO W, ASIF M, NAZEER W. The study of honey comb derived network via topological indices [J]. Open Journal of Mathematical Sciences, 2017, 2 (2): 10 - 26.