On the general zeroth-order Randić index of bargraphs

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Abstract

In this paper, we study the bargraphs in the perspective of a well-known topological index, namely the general zeroth-order Randić index. More precisely, we show that the expected value of the general zeroth-order Randić index over all bargraphs with n cells is $\frac{n}{3}(3^{\alpha+1} + 2^{\alpha} + 3 \cdot 2^{2\alpha-1})$ when n is large enough, where α is a non-zero real number.

Keywords: bargraphs; generating functions; topological index; general zeroth-order Randić index; general first Zagreb index.

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1. Introduction

In graph theory, an invariant of a graph is a numerical quantity that depends only on its abstract structure, not on graph representations such as particular labeling or drawing of the graph. A topological index is an invariant of a molecular graph associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. Nowadays, there exists a legion of topological indices with some applications in chemistry, especially in QSAR (quantitative structure-activity relationship) and QSPR (quantitative structure-property relationship) studies [18]. Since topological indices have gained considerable popularity recently, many new topological indices have been proposed and studied in the mathematical chemistry literature.

In 1975, Randić introduced the connectivity index [17], which is one of the the most studied and applied topological indices in QSPR and QSAR researches, defined by

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}},$$

where deg(u) and deg(v) denote the degree of the vertices u and v, respectively. Gutman and Trinajstić [9] derived a formula where the following topological index was appeared

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2.$$

The topological index M_1 is nowadays known as the first Zagreb index. Li and Zheng [11] generalized the concept of the first Zagreb index

$$M_1^{\alpha}(G) = \sum_{u \in V(G)} \deg(u)^{\alpha},$$

where α is a non-zero real number. The topological index M_1^{α} is also known as the general zeroth-order Randić index and also it is denoted by ${}^{0}R_{\alpha}$. It is easy to see that, for each value of α , there is a corresponding topological index. For instance, we get for $\alpha = -2$, the modified first Zagreb index [15]; for $\alpha = -1$, the inverse degree [6]; for $\alpha = -\frac{1}{2}$, zeroth-order Randić index [10]; and for $\alpha = 2, 3$, the first Zagreb index, forgotten topological index [9], respectively. Further detail about the general zeroth-order Randić index can be found in a recent survey [1].

The aim of this paper is to study ${}^{0}R_{\alpha}(G)$ for the case when G is a graph corresponding to a bargraph. A bargraph is a column-convex polyomino, drawn on a regular planar lattice and is made up of square cells such that the lower edge lies on the horizontal *x*-axis. Clearly, the number of parts and the size of the composition is the number of columns and the total number of cells in the representing bargraph, respectively. For instance, Figure 1 represents the bargraph 12234131.

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Bargraphs (see, e.g., [7,8]) have been studied from different points of views. For instance, the generating function for the number of bargraphs according to the number of horizontal and up steps is calculated in [7,16]. Blecher et al. obtained some other enumerative results related to bargraphs by counting them according to some statistics such as descents [4], levels [2], peaks [3] and walls [5]. Moreover, in [14] (see also, [12]) bargraphs were counted according to the number of interior vertices. The generating function for the number of bargraphs according to the area, the number of border cells and the number of tangent cells was studied in [13].

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Figure 1: The bargraph 12234131.

For any real number α , we define $N_{\alpha}(\pi) = {}^{0}R_{\alpha}(G_{\pi})$, where G_{π} is the graph represented by the bargraph π . In this note, we will show that the expected value of N_{α} over all bargraphs with n cells, when n is large enough, is

$$\frac{n}{3}(3^{\alpha+1} + 2^{\alpha} + 3 \cdot 2^{2\alpha-1})$$

2. Main results

We denote the set of all bargraphs with n cells by \mathcal{B}_n . For any bargraph $\pi \in \mathcal{B}_n$, we denote the number of columns of π by $col(\pi)$. Moreover, we denote the number of vertices in G_{π} with degree j by $deg_j(\pi)$. Clearly, $deg_j(\pi) = 0$ for any $j \ge 5$ and j = 1. For instance, Figure 1 demonstrates a bargraph $\pi = 12234131$ with $col(\pi) = 8$, $deg_1(\pi) = 0$, $deg_2(\pi) = 10$, $deg_3(\pi) = 12$ and $deg_4(\pi) = 10$. Define

$$B_n(y) = \sum_{\pi \in \mathcal{B}_n} y^{col(\pi)} \prod_{j=2}^4 q_j^{deg_j(\pi)}$$

and

$$B(x,y) = \sum_{n \ge 0} B_n(y) x^n,$$

where the variables x, y, q_1, q_2, q_3, q_4 are indeterminates. In order to study B(x, y), we refine it as

$$B(x, y|b_1 b_2 \cdots b_s) = \sum_{n \ge 0} \sum_{\pi = b_1 b_2 \cdots b_s \pi' \in \mathcal{B}_n} y^{col(\pi)} x^n \prod_{j=2}^4 q_j^{deg_j(\pi)}$$

By definitions, we have

$$B(x,y) = 1 + \sum_{a \ge 1} B(x,y|a)$$

Moreover, since each bargraph with the size of the first column being *a* can be written as either *a*, $ab\pi'$ with $1 \le b \le a-1$, $aa\pi'$ or $ab\pi'$ with $b \ge a+1$, where π' is any bargraph, we have

$$\begin{split} B(x,y|a) &= xyq_2^4 q_3^{2(a-1)} + \sum_{b\geq 1} B(x,y|ab) \\ &= x^a yq_2^4 q_3^{2(a-1)} + x^a y \sum_{b=1}^{a-1} q_2 q_3^{2a-2b} q_4^b B(x,y|b) \\ &\quad + x^a yq_3^2 q_4^{a-1} B(x,y|a) + x^a yq_2 q_4^a \sum_{b\geq a+1} B(x,y|b), \end{split}$$

where $a \ge 1$. Define

$$B(x, y, v) = 1 + \sum_{a \ge 1} B(x, y|a)v^{a-1}.$$

By multiplying the recurrence relation by v^{a-1} and summing over $a \ge 1$, we obtain

$$B(x, y, v) = 1 + \frac{xyq_2^4}{1 - vxq_3^2} + \frac{vx^2yq_2q_3^2q_4}{1 - vxq_3^2}(B(x, y, vxq_4) - 1) + xyq_3^2(B(x, y, q, vxq_4) - 1) + \frac{xyq_2q_4}{1 - vxq_4}(B(x, y, 1) - B(x, y, vxq_4)).$$

If we define

$$f(v) = \frac{xyq_2^4}{1 - vxq_3^2} + \frac{xyq_2q_4}{1 - vxq_4}(B(x, y, 1) - 1)$$

and

$$g(v) = \frac{vxq_2q_3^2q_4}{1 - vxq_3^2} + q_3^2 - \frac{q_2q_4}{1 - vxq_4},$$

then we have

$$B(x, y, v) - 1 = f(v) + xyg(v)(B(x, y, vxq_4) - 1).$$

By iterating last equation (here we assume that |x|, |y| < 1), we obtain

$$B(x, y, v) - 1 = \sum_{j \ge 0} x^j y^j f(v x^j q_4^j) \prod_{i=0}^{j-1} g(v x^i q_4^i),$$

which is equivalent to

$$B(x,y,v) - 1 = q_2 \sum_{j \ge 1} x^j y^j \left(\frac{q_2^3}{1 - v x^j q_4^{j-1} q_3^2} + \frac{q_4(B(x,y,1) - 1)}{1 - v x^j q_4^j} \right) \prod_{i=1}^{j-1} \left(\frac{v x^i q_2 q_3^2 q_4^i}{1 - x^i q_4^{i-1} q_3^2} + q_3^2 - \frac{q_2 q_4}{1 - v x^i q_4^i} \right)$$

By substituting v = 1 and solving for B(x, y, 1), with using the fact that B(x, y) = B(x, y, 1), we obtain the following result. **Theorem 2.1.** *The generating function* B(x, y) *is given by*

$$B(x,y) = 1 + \frac{q_2^4 \sum_{j \ge 1} \frac{x^j y^j}{1 - x^j q_4^{j-1} q_3^2} \prod_{i=1}^{j-1} \left(\frac{x^i q_2 q_3^2 q_4^i}{1 - x^i q_4^{i-1} q_3^2} + q_3^2 - \frac{q_2 q_4}{1 - x^i q_4^i} \right)}{1 - q_2 q_4 \sum_{j \ge 1} \frac{x^j y^j}{1 - x^j q_4^j} \prod_{i=1}^{j-1} \left(\frac{x^i q_2 q_3^2 q_4^i}{1 - x^i q_4^{i-1} q_3^2} + q_3^2 - \frac{q_2 q_4}{1 - x^i q_4^i} \right)}$$

Theorem 2.1 with $q_j = q^{j^{\alpha}}$ for j = 2, 3, 4 and y = 1 gives the following corollary.

Corollary 2.1. Define

$$F(x,q) = \sum_{n \ge 0} \sum_{\pi \in \mathcal{B}_n} q^{N_\alpha(\pi)} x^n$$

Then

$$F(x,q) = 1 + \frac{q^{4 \cdot 2^{\alpha}} \sum_{j \ge 1} \frac{x^{j}}{1 - x^{j} q^{(j-1)4^{\alpha} + 2 \cdot 3^{\alpha}}} \prod_{i=1}^{j-1} \left(\frac{x^{i} q^{2^{\alpha} + 2 \cdot 3^{\alpha} + i4^{\alpha}}}{1 - x^{i} q^{(i-1)4^{\alpha} + 2 \cdot 3^{\alpha}}} + q^{2 \cdot 3^{\alpha}} - \frac{q^{2^{\alpha} + 4^{\alpha}}}{1 - x^{i} q^{i4^{\alpha}}} \right)}{1 - q^{2^{\alpha} + 4^{\alpha}} \sum_{j \ge 1} \frac{x^{j}}{1 - x^{j} q^{j4^{\alpha}}} \prod_{i=1}^{j-1} \left(\frac{x^{i} q^{2^{\alpha} + 2 \cdot 3^{\alpha} + i4^{\alpha}}}{1 - x^{i} q^{(i-1)4^{\alpha} + 2 \cdot 3^{\alpha}}} + q^{2 \cdot 3^{\alpha}} - \frac{q^{2^{\alpha} + 4^{\alpha}}}{1 - x^{i} q^{i4^{\alpha}}} \right)}}$$

Corollary 2.1 for q = 1 gives

$$F(x,1) = 1 + \frac{\sum_{j\geq 1} \frac{x^j}{1-x^j} \prod_{i=1}^{j-1} \left(\frac{x^i}{1-x^i} + 1 - \frac{1}{1-x^i}\right)}{1 - \sum_{j\geq 1} \frac{x^j}{1-x^j} \prod_{i=1}^{j-1} \left(\frac{x^i}{1-x^i} + 1 - \frac{1}{1-x^i}\right)}$$
$$= 1 + \frac{x/(1-x)}{1-x/(1-x)} = \frac{1-x}{1-2x},$$

as expected.

Now we are ready to find an explicit formula for $\sum_{\pi \in \mathcal{B}_n} N_{\alpha}(\pi)$, that is, the sum of the general zeroth-order Randić indices over all bargraphs with *n* cells. By differentiating F(x,q) with respect to *q* and evaluating it at q = 1, we obtain

$$\frac{\partial}{\partial q}F(x,q)_{|q=1} = \frac{\partial}{\partial q} \left(\frac{\frac{q^{4\,2^{\alpha}}x}{1-xq^{2\,3^{\alpha}}} + q^{4\,2^{\alpha}}x^{2}\frac{\frac{xq^{2^{\alpha}+2\,3^{\alpha}+4^{\alpha}}}{1-xq^{2\,3^{\alpha}}} + q^{2\,3^{\alpha}} - \frac{q^{2^{\alpha}+4^{\alpha}}}{1-xq^{4^{\alpha}+2\,3^{\alpha}}}}{1-x^{2}q^{4^{\alpha}+2\,3^{\alpha}} + q^{2\,3^{\alpha}+2^{3^{\alpha}+4^{\alpha}}}}{1-x^{2}q^{2^{\alpha}+2,3^{\alpha}+4^{\alpha}}}} \right)_{|q=1} = \frac{x\left(2\,x^{3}3^{\alpha} - 6\,x^{3}2^{\alpha} + x^{3}4^{\alpha} + 4\,x^{2}3^{\alpha} + 2^{1+\alpha}x^{2} - 2\,4^{\alpha}x^{2} - 4\,3^{\alpha}x + 8\,2^{\alpha}x - 4\,2^{\alpha}\right)}{(x^{2}-1)\left(1-2\,x\right)^{2}}$$

Hence, we can state the following result.

Corollary 2.2. The sum of the general zeroth-order Randić indices over all bargraphs with n cells, $\sum_{\pi \in \mathcal{B}_n} N_{\alpha}(\pi)$, is given by

$$\frac{1}{36}(31 \cdot 2^{\alpha+1} - 21 \cdot 2^{2\alpha} + 2 \cdot 3^{\alpha+1} + 2 \cdot 3^{\alpha+2}n + 3n \cdot 2^{\alpha+1} + 9n \cdot 2^{2\alpha})2^n + \frac{1}{36}(4 \cdot 3^{\alpha+1} - 2^{\alpha+3} - 3 \cdot 2^{2\alpha+1})(-1)^n - 3^\alpha + 2^{2\alpha-1}.$$

Moreover, the expected value of the general zeroth-order Randić index over all bargraphs with n cells, when n is large enough, is given by

$$\frac{n}{3}(3^{\alpha+1}+2^{\alpha}+3\cdot 2^{2\alpha-1}).$$

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