M-Polynomial Revisited: Bethe Cacti and an Extension of Gutman's Approach

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Abstract

The M-polynomial of a graph G is defined as $\sum_{i\le j} m_{i,j}(G)x^i y^j$, where $m_{i,j}(G)$, $i,j\ge 1$, is the number of edges uv of G such that $\{d_v(G), d_u(G)\} = \{i,j\}$. Knowing the M-polynomial, formulas for bond incident degree indices (an important subclass of degree-based topological indices) can be obtained by means of specific operators defined on differentiable functions in two variables. This is illustrated on three infinite families of Bethe cacti. Gutman's approach for the computation of the coefficients of the M-polynomial is also recalled and an extension of it is given. This extension is used to determine the M-polynomial of a two-parameter infinite family of lattice graphs.

Keywords: M-polynomial; Bethe cacti; degree-based topological index; bond incident degree index; graph polynomial.

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1 Introduction

A large part of chemical graph theory investigates topological indices (in other words, graph invariants) which are aimed to be chemically relevant. Among these topological indices, degree-based ones, such as different variants of the Randić index and the Zagreb index, play a central role. For a general and uniform discussion on the degree-based topological indices see the survey [12]. For selected recent investigations of (variants of) the Randić index see [5, 6, 20, 21] and for (variants of) the Zagreb index we refer to [2, 29, 30]. We also refer to [13], where these

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indices are correlated with physico-chemical parameters of octane isomers. For a selection of recent papers that compute degree-based topological indices see [1, 16, 17, 19, 22, 23, 24, 25]; we especially emphasize the approach to degree-based topological indices of hexagonal nanotubes in [27].

In order to simplify the computation of the bond incident degree indices, which form an utmost important subclass of degree-based topological indices (to be defined in Section 2), and to stop the production of papers that, for a given family of graphs computes a given topological index from skratch, the M-polynomial was introduced in [8]. (For a related approach using the degree sequence polynomial for generalized Zagreb indices, see [9].) In [8] it was proved that the computation of several degree-based topological indices becomes a routine task, provided that the corresponding M-polynomial is known. More precisely, the problem more or less reduces to the one of determining the number $m_{i,j}$ of the edges of a graph whose endpoints are of degrees i and j. Hence a particular purpose of this paper is to point out to future authors that

(i) the expressions for the $m_{i,j}$s should be derived (or explained) and that

(ii) not much space should be taken up by the computation of the topological indices; they follow easily either by elementary algebra from the $m_{i,j}$s or by elementary calculus from the M-polynomial.

Numerous very recent papers that compute degree-based topological indices do not satisfy these natural requirements. Therefore, in this paper we further explain the approach and demonstrate its power on three families of Bethe cacti from [3]. These families have been selected in particular because the determination of the M-polynomial (equivalently of the corresponding $m_{i,j}$s) is not that straightforward as it is in several earlier cases.

The rest of the paper is organized as follows. In the next section we formally introduce the M-polynomial and recall how it can be applied to bond incident degree topological indices. In Section 3 we introduce three families of Bethe cacti, give their recursive definitions, and based on them determine the M-polynomial in all of the cases. In Section 4 we combine the results from the previous two sections to give closed formulas for several degree-based topological indices of the considered Bethe cacti. In the concluding section we recall Gutman's approach for the computation of the coefficients of the M-polynomial. We extend this approach by adjoining Euler's formula to the original six equalities. We use this extended approach to determine the M-polynomial of a two-parameter infinite family of lattice graphs, consisting of 5-, 6-, and 8-gonal faces.

We do not give basic definitions of graph theory here; the reader can consult the book [31].

2 Preliminaries

Let $G = (V(G), E(G))$ be a graph and let $m_{i,j}(G)$, $i, j \geq 1$, be the number of edges uv of G such that $\{d_v(G), d_u(G)\} = \{i, j\}$, where $d_v(G)$ (or d_v for short) is the degree of the vertex v in G. (It seems that the variables $m_{i,j}$ were introduced for the first time in [11].) For instance, if G is k-regular, then $m_{k,k} = |E(G)|$, while $m_{i,j}(G) = 0$ as soon as $i \neq k$ or $j \neq k$. The *M-polynomial* of G is the two variable polynomial defined as

$$\sum_{i \leq j} m_{i,j}(G) x^i y^j \,.$$

The role of this polynomial for degree-based indices is similar to the role of the Hosoya polynomial [15] (see also [7, 10, 18, 26]) for distance-based invariants.

A *degree-based topological index* I of a graph G is an arbitrary graph invariant that is defined as a function of the degrees of the vertices of G. In many important cases, I is of the form

$$I(G) = \sum_{e=uv \in E} f(d_u, d_v)\,, \tag{1}$$

where $f = f(x, y)$ is a function to be suitable for chemical applications [12, 14]. The degree-based topological indices I that are of the form (1) were named *bond incident degree indices* in [28]; we follow this terminology here. We will also abbreviate bond incident degree index to *BID index*. For instance, the generalized Randić index $R_\alpha(G)$, $\alpha \neq 0$, is a BID index because it is obtained by selecting $f(x, y) = (xy)^\alpha$ [4]; see Table 1 for additional important BID indices. As examples of degree-based topological indices that are not BID indices consider the higher order Randić indices. In this case the summation is taken over all paths in a graph of a given length instead over all edges as it is done in (1).

From our point of view it is utmost important to note that (1) can be rewritten as

$$I(G) = \sum_{i \leq j} m_{i,j}(G) f(i, j)\,. \tag{2}$$

Consider the following operators defined on differentiable functions in two variables:

$$\begin{aligned} D_x(f(x,y)) &= x\tfrac{\partial f(x,y)}{\partial x}, & D_y(f(x,y)) &= y\tfrac{\partial f(x,y)}{\partial y}, \\ S_x(f(x,y)) &= \textstyle\int_0^x \frac{f(t,y)}{t}dt, & S_y(f(x,y)) &= \textstyle\int_0^y \frac{f(x,t)}{t}dt, \\ J(f(x,y)) &= f(x,x), & Q_\alpha(f(x,y)) &= x^\alpha f(x,y), \alpha \neq 0. \end{aligned}$$

Now we can recall the following key result from [8].

Theorem 2.1 [8, Theorems 2.1,2.2] *Let G be a graph.*

(i) *If* $I(G) = \sum_{e=uv\in E} f(d_u, d_v)$, *where* $f(x,y)$ *is a polynomial in* x *and* y, *then*

$$I(G) = f(D_x, D_y)(M(G;x,y))\big|_{x=y=1}\,.$$

(ii) *If* $I(G) = \sum_{e=uv\in E} f(d_u, d_v)$, *where* $f(x,y) = \sum_{i,j\in\mathbb{Z}} \alpha_{ij} x^i y^j$, *then* $I(G)$ *can be obtained from* $M(G;x,y)$ *using the operators* D_x, D_y, S_x, *and* S_y.

(iii) *If* $I(G) = \sum_{e=uv\in E} f(d_u, d_v)$, *where* $f(x,y) = \frac{x^r y^s}{(x+y+\alpha)^k}$, *where* $r, s \geq 0$, $, t \geq 1$, *and* $\alpha \in \mathbb{Z}$, *then*

$$I(G) = S_x^k\, Q_\alpha\, J\, D_x^r\, D_y^s (M(G;x,y))\big|_{x=1}\,.$$

Table 1 contains applications of Theorem 2.1 for some of the main BID indices.

BID index	$f(x,y)$	derivation from $M(G;x,y)$
first Zagreb	$x+y$	$(D_x + D_y)(M(G;x,y))\big\|_{x=y=1}$
second Zagreb	xy	$(D_x D_y)(M(G;x,y))\big\|_{x=y=1}$
second modified Zagreb	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y))\big\|_{x=y=1}$
general Randić ($\alpha \in \mathbb{N}$)	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\big\|_{x=y=1}$
general Randić ($\alpha \in \mathbb{N}$)	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\big\|_{x=y=1}$
symmetric division index	$\frac{x^2+y^2}{xy}$	$(D_x S_y + D_y S_x)(M(G;x,y))\big\|_{x=y=1}$
harmonic	$\frac{2}{x+y}$	$2\, S_x\, J\,(M(G;x,y))\big\|_{x=1}$
inverse sum	$\frac{xy}{x+y}$	$S_x\, J\, D_x\, D_y\,(M(G;x,y))\big\|_{x=1}$
augmented Zagreb	$\left(\frac{xy}{x+y-2}\right)^3$	$S_x^3\, Q_{-2}\, J\, D_x^3\, D_y^3\,(M(G;x,y))\big\|_{x=1}$

Table 1: How to compute important BID indices from the M-polynomial

3 Families of Bethe cacti

Balasubramanian [3] considered families C_n, D_n, and E_n ($n \geq 1$) of cactus graphs. Since the recursive structure of the families C_n and E_n can be described using the family D_n, we first consider the family D_n.

3.1 Bethe cacti D_n

The recursive definition of the family of the Bethe cacti D_n, $n \geq 1$, is shown in Fig. 1. Here the black vertex of D_n denotes the attaching vertex, where D_n is attached to D_{n+1} (three times).

The smallest Bethe cactus D_1 is shown in the recursive description (Fig. 1), while the next two Bethe cacti D_2 and D_3 are drawn in Fig. 2. The general construction should then be clear.

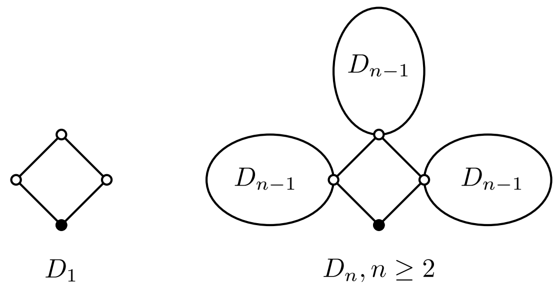

Figure 1: Recursive definition of the Bethe cacti D_n

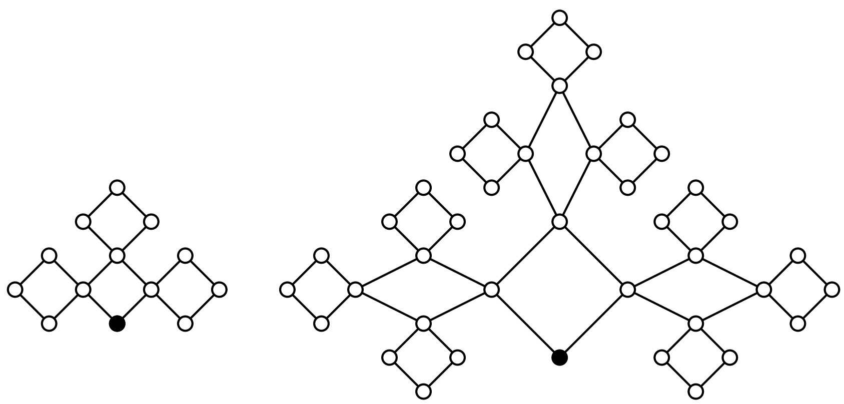

Figure 2: The Bethe cacti D_2 and D_3

Theorem 3.1 *$M(D_1; x, y) = 4x^2y^2$ and if $n \geq 2$, then*

$$M(D_n; x, y) = 2 \cdot 3^{n-1}x^2y^2 + 2(3^{n-1} + 1)x^2y^4 + 2(3^{n-1} - 2)x^4y^4 \, .$$

Proof. Clearly, $M(D_1; x, y) = 4x^2y^2$. Assume in the rest that $n \geq 2$ and for the initial condition in the following three recurrences consider D_2 from Fig. 2. We first infer that

$$m_{2,2}(D_2) = 6, \quad m_{2,2}(D_n) = 3m_{2,2}(D_{n-1}), n \geq 3 \, ,$$

which solves as $m_{2,2}(D_n) = 2 \cdot 3^{n-1}$.

Note further that two 24-edges of D_{n-1} become 44-edges in D_n. Consequently,

$$m_{2,4}(D_2) = 8, \quad m_{2,4}(D_n) = 3m_{2,4}(D_{n-1}) - 6 + 2, n \geq 3 \, ,$$

which solves into $m_{2,4}(D_n) = 2 \cdot 3^{n-1} + 2$ and

$$m_{4,4}(D_2) = 2, \quad m_{4,4}(D_n) = 3m_{4,4}(D_{n-1}) + 6 + 2, n \geq 3\,,$$

which in turn solves into $m_{4,4}(D_n) = 2 \cdot 3^{n-1} - 4$. Putting together the three solutions of the recurrences, the result follows. □

3.2 Bethe cacti C_n

The recursive definition of the family of the Bethe cacti C_n, $n \geq 1$, is shown in Fig. 3. The vertex at which each of the four copies of D_{n-1} is attached to the central 4-cycle, respectively, is the black vertex of D_{n-1} as shown in Fig. 2. The smallest Bethe cactus C_1 is thus the 4-cycle graph, while the Bethe cacti C_2 and C_3 are drawn in Fig. 4. The general construction should then be clear.

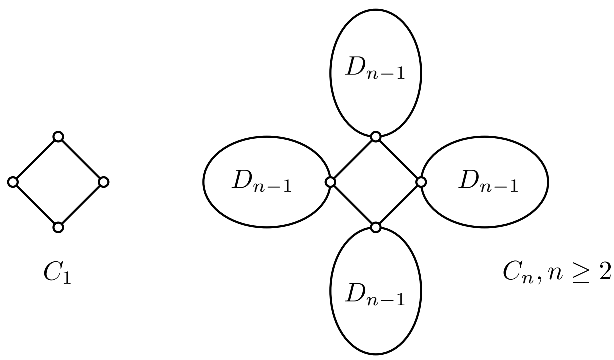

Figure 3: Recursive definition of the Bethe cacti C_n

Theorem 3.2 *$M(C_1; x, y) = 4x^2y^2$ and if $n \geq 2$, then*

$$M(C_n; x, y) = 8 \cdot 3^{n-2}x^2y^2 + 8 \cdot 3^{n-2}x^2y^4 + 4(2 \cdot 3^{n-2} - 1)x^4y^4\,.$$

Proof. Clearly, $M(C_1; x, y) = 4x^2y^2$. Assume in the rest that $n \geq 2$. Recalling from the proof of Theorem 3.1 that $m_{2,2}(D_n) = 2 \cdot 3^{n-1}$, we have

$$m_{2,2}(C_n) = 4m_{2,2}(D_{n-1}) = 4 \cdot 2 \cdot 3^{n-2} = 8 \cdot 3^{n-2}\,.$$

Recalling further that $m_{2,4}(D_n) = 2 \cdot 3^{n-1} + 2$ and $m_{4,4}(D_n) = 2 \cdot 3^{n-1} - 4$, and observing that two 24-edges of D_{n-1} become 44-edges in C_n, we get

$$m_{2,4}(C_n) = 4m_{2,4}(D_{n-1}) - 8 = 4(2 \cdot 3^{n-2} + 2) - 8 = 8 \cdot 3^{n-2}$$

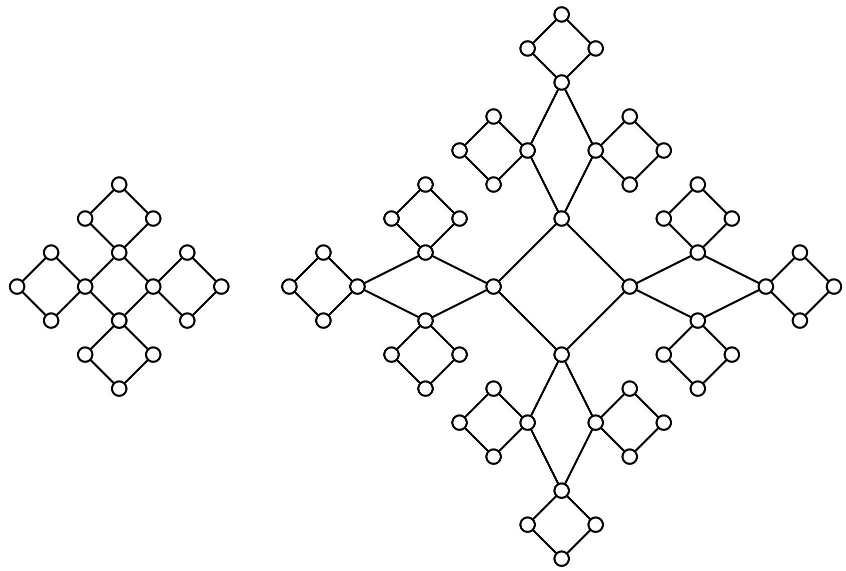

Figure 4: The Bethe cacti C_2 and C_3

and

$$m_{4,4}(C_n) = 4m_{4,4}(D_{n-1}) + 8 + 4 = 4(2 \cdot 3^{n-2} - 4) + 12 = 8 \cdot 3^{n-2} - 4\,.$$

Hence the result. □

3.3 Bethe cacti E_n

The recursive definition of the family of the Bethe cacti E_n, $n \geq 1$, is shown in Fig. 5. Again, the vertex at which each of the three copies of D_{n-1} is attached to the central path on three vertices, respectively, is the black vertex of D_{n-1} as shown in Fig. 2. Thus the smallest Bethe cactus E_1 is the path on three vertices, the next two Bethe cacti E_2 and E_3 are drawn in Fig. 6. The general construction should then be clear.

Theorem 3.3 $M(E_1; x, y) = 2xy^2$, $M(E_2; x, y) = 6x^2y^2 + 4x^2y^3 + 2x^2y^4 + 2x^3y^4$, *and if* $n \geq 3$, *then*

$$M(E_n; x, y) = 2 \cdot 3^{n-1}x^2y^2 + 2 \cdot 3^{n-1}x^2y^4 + 6x^3y^4 + (2 \cdot 3^{n-1} - 10)x^4y^4\,.$$

Proof. Clearly, $M(E_1; x, y) = 2xy^2$ and $M(E_2; x, y) = 6x^2y^2 + 4x^2y^3 + 2x^2y^4 + 2x^3y^4$. Assume in the rest that $n \geq 3$. Note that two 24-edges of the middle D_{n-1} become 44-edges in E_n, and that two 24-edges of an extreme D_{n-1} become 34-edges in E_n. Hence, recalling again from the proof

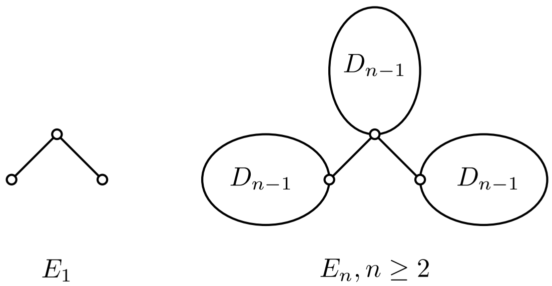

Figure 5: Recursive definition of the Bethe cacti E_n

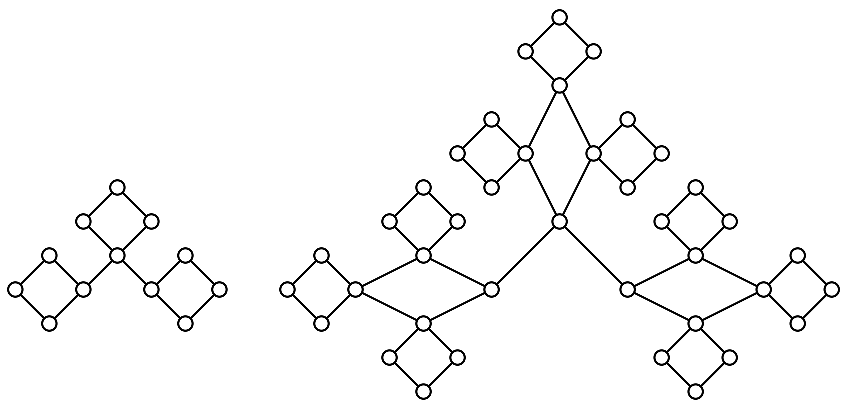

Figure 6: The Bethe cacti E_2 and E_3

of Theorem 3.1 that $m_{2,2}(D_n) = 2 \cdot 3^{n-1}$, $m_{2,4}(D_n) = 2 \cdot 3^{n-1} + 2$, and $m_{4,4}(D_n) = 2 \cdot 3^{n-1} - 4$, we get:

$$\begin{aligned}
m_{2,2}(E_n) &= 3m_{2,2}(D_{n-1}) = 3 \cdot 2 \cdot 3^{n-2} = 2 \cdot 3^{n-1}\,, \\
m_{2,3}(E_n) &= 3m_{2,3}(D_{n-1}) = 0\,, \\
m_{2,4}(E_n) &= 3m_{2,4}(D_{n-1}) - 6 = 3 \cdot 2 \cdot 3^{n-2} + 6 - 6 = 2 \cdot 3^{n-1}\,, \\
m_{3,3}(E_n) &= 3m_{3,3}(D_{n-1}) = 0\,, \\
m_{3,4}(E_n) &= 3m_{3,4}(D_{n-1}) + 4 + 2 = 6\,, \\
m_{4,4}(E_n) &= 3m_{4,4}(D_{n-1}) + 2 = 3 \cdot 2 \cdot 3^{n-2} - 12 + 2 = 2 \cdot 3^{n-1} - 10\,.
\end{aligned}$$

Putting all this together, the result follows. □

4 Topological indices of Bethe cacti

Combining Theorem 3.1 with the expressions from Table 1, routine computations yield the expressions for the selected listed topological indices of D_n, C_n, and E_n, $n \geq 2$. Let us demonstrate this by computing the symmetric division index of D_n, $n \geq 2$. From Table 1 we know that this reduces to compute $(D_xS_y + D_yS_x)(M(G;x,y))\big|_{x=y=1}$. Now,

$$\begin{aligned} S_x(M(D_n;x,y)) &= \int_0^x \frac{2 \cdot 3^{n-1}t^2y^2 + 2(3^{n-1}+1)t^2y^4 + 2(3^{n-1}-2)t^4y^4}{t} \\ &= \frac{3^{n-1}x^2y^2(x^2y^2 + 2(y^2+1))}{2} - x^4y^4 + x^2y^4 \,, \end{aligned}$$

and hence

$$D_yS_x(M(D_n;x,y)) = y \cdot (2 \cdot 3^{n-1}x^2y(x^2y^2 + 2y^2 + 1) - 4x^2y^3(x^2-1)) \,. \tag{3}$$

Similarly we compute that

$$D_xS_y(M(D_n;x,y)) = x \cdot (3^{n-1}xy^2(2x^2y^2 + y^2 + 2) - xy^4(4x^2-1)) \,. \tag{4}$$

Summing (3) and (4) we get

$$(D_xS_y + D_yS_x)(M(G;x,y)) = 3^{n-1}x^2y^2(4x^2y^2 + 5y^2 + 4) - x^2y^4(8x^2 - 5)$$

from where we conclude that

$$(D_xS_y + D_yS_x)(M(G;x,y))\big|_{x=y=1} = 13 \cdot 3^{n-1} - 3 \,.$$

All the other entries from Table 2 are computed along the same lines.

topological index I	$I(D_n)$	$I(C_n)$	$I(E_n)$
first Zagreb	$4 \cdot 3^{n+1} - 20$	$16 \cdot 3^n - 32$	$4 \cdot 3^{n+1} - 38$
second Zagreb	$56 \cdot 3^{n-1} - 48$	$224 \cdot 3^{n-2} - 64$	$56 \cdot 3^{n-1} - 88$
second modified Zagreb	$\frac{7}{8} \cdot 3^{n-1}$	$\frac{7}{2} \cdot 3^{n-2} - \frac{1}{4}$	$\frac{7}{8} \cdot 3^{n-1} - \frac{1}{8}$
symmetric division index	$13 \cdot 3^{n-1} - 3$	$52 \cdot 3^{n-2} - 8$	$13 \cdot 3^{n-1} - \frac{15}{2}$
harmonic	$\frac{13}{2} \cdot 3^{n-2} - \frac{1}{3}$	$26 \cdot 3^{n-3} - 1$	$\frac{13}{2} \cdot 3^{n-2} - \frac{11}{14}$
inverse sum	$26 \cdot 3^{n-2} - \frac{16}{3}$	$104 \cdot 3^{n-3} - 8$	$26 \cdot 3^{n-2} - \frac{68}{7}$

Table 2: Selected topological indices of Bethe cacti

5 (An extension of) Gutman's approach

As already pointed out in [8], an approach to determine the coefficients $m_{i,j}$ of an M-polynomial has been proposed by Gutman [11] by considering corresponding linear equations. Let us briefly recall the approach here, in particular to correct a statement from [8, p. 99] (see below).

Let G be a chemical graph (a graph of maximum degree at most 4) with n vertices and m edges, and let n_i, $1 \leq i \leq 4$, be the number of vertices of degree i. Clearly, $m_{1,1} = 0$ as soon as the graph has at least three vertices and is connected, while for the the other $m_{i,j}$s we have:

$$\begin{aligned} n_1 + n_2 + n_3 + n_4 &= n && (5) \\ m_{1,2} + m_{1,3} + m_{1,4} &= n_1 && (6) \\ m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} &= 2n_2 && (7) \\ m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} &= 3n_3 && (8) \\ m_{1,4} + m_{2,4} + m_{3,4} + 2m_{4,4} &= 4n_4 && (9) \\ n_1 + 2n_2 + 3n_3 + 4n_4 &= 2m\,. && (10) \end{aligned}$$

Equations (5)-(9) are linearly independent, while (10) is a consequence of (5)-(9). (In [8] it is said that all these equations are linearly independent.) Gutman's approach is to determine first some of the $m_{i,j}$s and then the remaining ones can be obtained from the above relations.

We extend Gutman's approach by adjoining to Equations (5)-(10) Euler's formula (cf. [31, p. 201])

$$\sum m_{i,j} - \sum n_i = f - 2\,, \tag{11}$$

usable whenever dealing with a plane graph whose number of faces f can be determined.

In the rest we are going to use this extended Gutman approach to determine the M-polynomial of the networks $G(p,q)$, $p,q \geq 1$. In Fig. 7 the network $G(3,4)$ is drawn, from which the general definition should be clear. In particular, $G(1,1)$ consists of an 8-gon with two 6-gons attached at the top and two 6-gons attached at the bottom.

Clearly, vertices of $G(p,q)$ are of degrees 2 and 3, hence we need to determine $m_{2,2} = m_{2,2}(G(p,q))$, $m_{2,3} = m_{2,3}(G(p,q))$, and $m_{3,3} = m_{3,3}(G(p,q))$.

Note first that

$$m_{2,2} = 2(p+1) + 4 = 2p + 6\,, \tag{12}$$

where $2(p+1)$ correspond the side edges with both end-points of degree 2, and 4 corresponds to the corner edges (with both end-points of degree 2). Furthermore, $n_2 = 4q + 4(p+1) + 2p = 6p + 4q + 4$, where $4q$ comes from the top and bottom vertices of degree 2, the term $4(p+1)$ comes from the sides, and the term $2p$ from the almost sides. Equation (7) in our case reduces

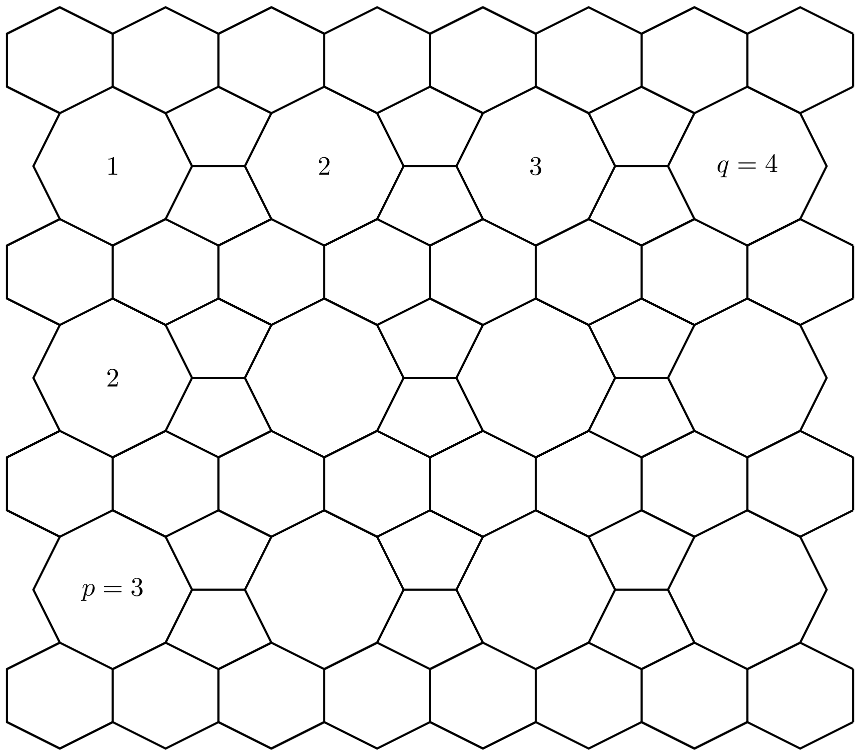

Figure 7: The lattice $G(3,4)$

to $2m_{2,2} + m_{2,3} = 2n_2$, from which we get

$$m_{2,3} = 8p + 8q - 4\,. \tag{13}$$

Equation (8) reduces to $m_{2,3} + 2m_{3,3} = 3n_3$ and therefore,

$$3n_3 - 2m_{3,3} = 8p + 8q - 4\,. \tag{14}$$

Since the number of 8-gons of $G(p,q)$ is pq, the number of its 6-gons is $2q(p+1)$, and the number of its 5-gons is $2p(q-1)$, Equation (11) reduces to

$$m_{3,3} - n_3 = 5pq - 6p - 2q + 1\,. \tag{15}$$

Solving (14) and (15) yields $n_3 = 10pq - 4p + 4q - 2$ and

$$m_{3,3} = 15pq - 10p + 2q - 1\,. \tag{16}$$

From Equations (12), (13), and (16) we conclude that

$$M(G(p,q);x,y) = (2p+6)x^2y^2 + (8p+8q-4)x^2y^3 + (15pq - 10p + 2q - 1)x^3y^3\,.$$

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