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How to Compute the M-Polynomial of (Chemical) Graphs

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Abstract

Let G be a graph and let $m_{i,j}(G)$, $i, j \geq 1$, be the number of edges uv of G such that $\{d_v(G), d_u(G)\} = \{i, j\}$. The M-polynomial of G is $M(G; x, y) = \sum_{i \leq j} m_{i,j}(G)x^i y^j$. A general method for calculating the M-polynomials for arbitrary graph families is presented. The method is further developed for the case where the vertices of a graph have degrees 2 and p, where $p \geq 3$, and further for such planar graphs. The method is illustrated on families of chemical graphs.

1 Introduction

Immediately after the M-polynomial was introduced in the paper [5], it received a lot of attention, which is still ongoing. The main reason for this popularity is the fact that as soon as we know this polynomial for a

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given graph family, we can routinely obtain closed formulas for a variety of degree-based topological indices on the family. Namely, computations can be translated to elementary calculus, see [5,6]. The list of papers [1–3, 14–17] is only a small part of the research in which the M-polynomial is a key tool used. A general approach to degree-based topological indices has been done in [10], while in [8] investigations of their structure-sensitivity in chemistry was performed. We also refer to the recent papers [4,9,11,12] in which extremal graphs with respect to degree-based indices are studied.

By the above, it is of key importance to develop methods for computing the M-polynomial. However, in the literature only sporadic, ad hoc methods can be found. One of the few more general attempts was presented in [7] where a method was proposed of how to determine the M-polynomial of planar, (chemical) graphs in which $d_G(v) \in \{2,3\}$ for each vertex v of G. The main goal of this paper is to extend this method to arbitrary graphs. We proceed as follows. In the rest of the introduction, the M-polynomial is formally introduced and some other needed definition is stated. In the next section we present a general method for calculating the M-polynomial of arbitrary graph families. In Section 3 the method is first specialized and further developed for the case where the vertices of a graph have degrees 2 and p, where $p \geq 3$. After that the method is restricted to planar graphs which are the source for the majority of chemical graphs of interest.

Let $G = (V(G), E(G))$ be a graph. The degree of a vertex $v \in V(G)$ will be denoted by $d_v(G)$ and the maximum degree of G by $\Delta(G)$. Further, we will use the following conventions:

- $n(G) = |V(G)|$ and $m(G) = |E(G)|$;
- $n_i(G)$, $i \geq 1$, is the number of vertices of G of degree i;
- for $i, j \geq 1$, $m_{i,j}(G) = |\{uv \in E(G) :\ \{d_v(G), d_u(G)\} = \{i,j\}\}|$.

Now, the *M-polynomial* of G is

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

2 The general method

In this section we present a general approach for determining the M-polynomial of an arbitrary graph. The main benefit of this approach is that we do not need to determine all $m_{i,j}$; instead we can express some of them with other graph invariants that are simpler to determine.

Let G be a connected graph with $n(G) \geq 3$. We may also assume in the rest that G is not regular, for otherwise its M-polynomial is trivial. For a fixed integer $i \geq 1$, consider all the vertices u of G of degree i and its incident edges. If uv is such an edge, then thus $d_G(u) = i$. Now, if $d_G(v) = j$, $j \neq i$, then the vertex u (via the edge uv) contributes 1 to $m_{i,j}$. On the other hand, if also $d_G(v) = i$, both vertices u and v contribute 1 to $m_{i,i}$. In consequence, $\sum_{j=1}^{\Delta(G)} m_{i,j} + m_{i,i} = 2n_i$ holds. Hence, the following equalities hold:

$$\sum_{i=1}^{\Delta(G)} n_i(G) = n(G),$$

$$\sum_{j=1}^{\Delta(G)} m_{i,j}(G) + m_{i,i}(G) = 2n_i(G),\ i \in [\Delta(G)], \tag{1}$$

$$\sum_{i=1}^{\Delta(G)} i \cdot n_i(G) = 2m(G),$$

where the first equality is obvious, the second equalities were justified above, and the last equality is a rewritten hand-shaking lemma. Note that since G is a connected graph on at least three vertices, $m_{1,1} = 0$.

Let k be the number of distinct elements in the degree sequence of G. Then the system (1) contains $\binom{k+1}{2} + k + 2$ variables and consists of $k + 2$ equations. Assuming the system has rank $k + 2$ (which will be the case in the following examples), we can select $\binom{k+1}{2}$ variables as parameters. They are selected among all the variables such that their direct computation is simplest among all the variables. Then the remaining "difficult" variables are determined by solving the system (1). Of course, we have to be careful that selected parameters do not produce linearly dependant systems. It turns out that at least one of $m_{i,j}$ must be known, otherwise the system cannot be solved.

It is clear that the described method is especially useful when the degree sequence contains few distinct values. We demonstrate this in the next section.

3 Graphs with degrees 2 and p

In this section, we restrict our attention to bi-degree graphs with degrees 2 and $p \geq 3$, that is, to graphs in which the degree sequence contains only values 2 and p. The special case $p = 3$ was studied earlier in [7]. We first consider general graphs and then specialize to planar graphs.

3.1 General graphs

Let G be a connected graph with vertices only of degrees 2 and p, where $p \geq 3$. Then (1) simplifies into:

$$\begin{aligned} n_2(G) + n_p(G) &= n(G), \\ 2m_{2,2}(G) + m_{2,p}(G) &= 2n_2(G), \\ m_{2,p}(G) + 2m_{p,p}(G) &= pn_p(G), \\ 2n_2(G) + pn_p(G) &= 2m(G). \end{aligned} \tag{2}$$

Our aim is to select three variables as parameters and solve the system for the other variables. We can not select all the three parameters from a single equation because this would remove one equation from the system and therefore we would not be able to solve it. Also we can not select $n(G)$, $m(G)$, and $n_2(G)$ as parameters since in this case the first and the last equation would became linearly dependant and again the system would be unsolvable. On the other hand, solving the system with parameters $n(G)$,

$m(G)$, and $m_{2,2}(G)$ yields the following solution:

$$\begin{aligned}
n_2(G) &= \frac{n(G)p - 2m(G)}{p-2}, \\
n_p(G) &= \frac{2(m(G) - n(G))}{p-2}, \\
m_{2,p}(G) &= \frac{n(G)p - 2m(G)}{p-2} - 2m_{2,2}(G), \\
m_{p,p}(G) &= m_{2,2}(G) + \frac{2n(G)p - m(G)(p+2)}{p-2}.
\end{aligned}$$

As a consequence we can state the following result, where $m_{i,j}(G)$ is simplified to $m_{i,j}$ and similarly all the other invariants of G.

Theorem 1. *If $p \geq 3$ and G is a connected graph with vertices only of degrees 2 and p, then*

$$\begin{aligned}
M(G; x, y) = m_{2,2}x^2y^2 &+ \left[\frac{np - 2m}{p-2} - 2m_{2,2}\right] x^2y^p \\
&+ \left[m_{2,2} + \frac{2np - m(p+2)}{p-2}\right] x^py^p \,.
\end{aligned}$$

For a concrete example, let X_n, $n \geq 1$, be the family of graphs inductively defined as follows. $X_1 = C_4$, and if $k \geq 2$, then X_k is obtained from X_{k-1} by attaching a pendant 4-cycle at every vertex of degree 2 of X_{k-1}. That is, to every vertex u of degree 2 of X_{k-1} we add a private 4-cycle and identify a vertex of the 4-cycle with u. See Fig. 1 where X_4 is shown.

By a direct computation we easily see that for $k \geq 1$ we have $n(X_k) = 2(3^k - 1)$ and $m(X_k) = 4(3^{k-1} - 1)$, and for $k \geq 2$ we have $n_{2,2}(X_k) = 8 \cdot 3^{k-2}$. Then Theorem 1 implies that for $k \geq 2$,

$$M(X_k; x, y) = 8 \cdot 3^{k-2}x^2y^2 + 8 \cdot 3^{k-2}x^2y^p + 4(2 \cdot 3^{k-2} - 1)x^py^p \,.$$

3.2 Planar graphs

In this subsection, G is a connected planar graph with vertices only of degrees 2 and p, where $p \geq 3$. The number of the faces in its plane embedding will be denoted by $f(G)$.

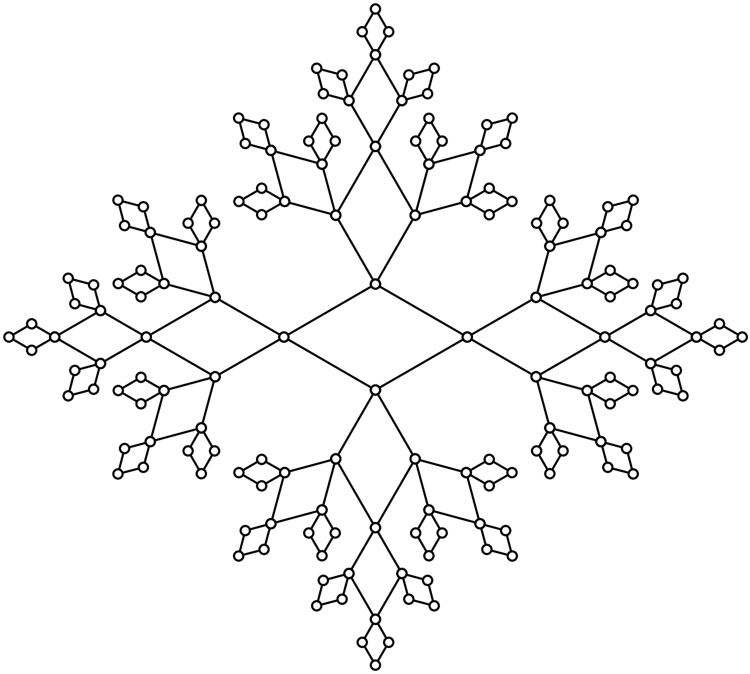

Figure 1. The graph X_4.

Now we can add the Euler formula to the system (2) and maintain independence property. Doing this we have added one additional equation and one additional variable to the system, hence we have a greater freedom to select three parameters. Let us now choose $n_2(G)$, $f(G)$, and $m_{2,2}(G)$ as the three parameters. Then the solution is:

$$\begin{aligned}
n(G) &= n_2(G) + \frac{2(f(G)-2)}{p-2}\\
m(G) &= n_2(G) + \frac{p(f(G)-2)}{p-2}\\
n_p(G) &= \frac{2(f(G)-2)}{p-2}\\
m_{2,p}(G) &= 2(n_2(G) - m_{2,2}(G))\\
m_{p,p}(G) &= m_{2,2}(G) - n_2(G) + \frac{p(f(G)-2)}{p-2}.
\end{aligned}$$

This gives the following result, where again the argument "(G)" is omitted for the sake of simplicity:

Theorem 2. *If $p \geq 3$ and G is a planar graph with vertices only of degrees 2 and p, then*

$$M(G;x,y) = m_{2,2}x^2y^2 + 2(n_2 - m_{2,2})x^2y^p + \left[m_{2,2} - n_2 + \frac{p(f-2)}{p-2}\right] x^py^p\,.$$

Plugging $p = 3$ into Theorem 2 we get the following previously known result.

Corollary. [7, Theorem 2.1] *If G is a planar graph with vertices only of degrees 2 and 3, and f is the number of faces of a plane embedding of G, then*

$$M(G;x,y) = m_{2,2}x^2y^2 + 2(n_2 - m_{2,2})x^2y^3 + (3f - n_2 + m_{2,2} - 6)x^3y^3\,.$$

Let next the parameters be $n_2(G)$, $n_p(G)$, and $m_{2,2}(G)$. Solving the system with these parameters yields:

$$\begin{aligned}
n(G) &= n_p(G) + n_2(G)\\
m(G) &= \frac{pn_p(G) + 2n_2(G)}{2}\\
m_{2,p}(G) &= 2(n_2(G) - m_{2,2}(G))\\
m_{p,p}(G) &= m_{2,2}(G) + \frac{pn_p(G) - 2n_2(G)}{2}\\
f(G) &= 2 - n_p(G) + \frac{pn_p(G)}{2}.
\end{aligned}$$

It is interesting to observe that the solution for the number of faces is only a function of the invariant $n_p(G)$ (and p). The corresponding result for the M-polynomial now reads as follows.

Theorem 3. *If G is a planar graph with vertices only of degrees 2 and p, where $p \geq 3$, then*

$$M(G;x,y) = m_{2,2}x^2y^2 + 2(n_2 - m_{2,2})x^2y^p + \left[m_{2,2} + \frac{pn_p - 2n_2}{2}\right] x^py^p\,.$$

4 Graphs with degrees 2, 3, and 4

In this section we demonstrate this method on certain zinc-based metal organic frameworks which contain vertices of degrees 2, 3, and 4. More precisely, we consider the molecular structures $Z(a,b)$, $a,b \geq 1$, the general definition should be clear from the example $Z(3,2)$ shown in Fig. 2.

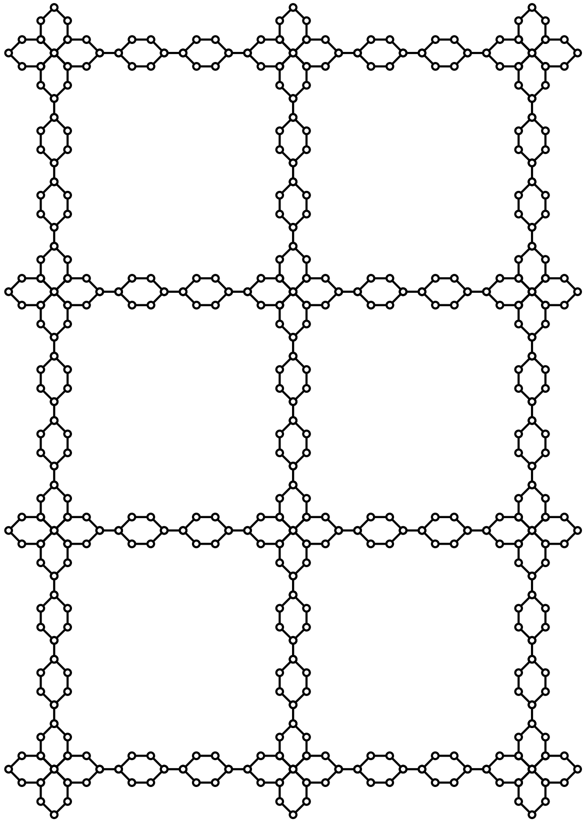

Figure 2. The graph $Z(3,2)$.

The molecular structures $Z(a,1)$ have been earlier considered in [13], where the corresponding M-polynomial was implicitly determined. Here we determine the M-polynomial for the general case $G = Z(a,b)$. The system (1) simplifies into the following, where $m_{2,4}(G) = m_{4,4}(G) = 0$ is used.

$$
\begin{aligned}
n_2(G) + n_3(G) + n_4(G) &= n(G), \\
2m_{2,2}(G) + m_{2,3}(G) &= 2n_2(G), \\
m_{2,3}(G) + 2m_{3,3}(G) + m_{3,4}(G) &= 3n_3(G), \\
m_{3,4}(G) &= 4n_4, \\
2n_2(G) + 3n_3(G) + 4n_4(G) &= 2m(G), \\
n(G) - m(G) + f(G) &= 2.
\end{aligned}
$$

Considering $n(G)$, $f(G)$, $n_4(G)$, and $m_{3,3}(G)$ as parameters, we get the following solution:

$$
\begin{aligned}
&m_{2,2}(G) = 6n_4(G) + m_{3,3}(G) + n(G) - 5f(G) + 10, \\
&m_{2,3}(G) = -10n_4(G) - 2m_{3,3}(G) + 6f(G) - 12, \\
&m_{3,4}(G) = 4n_4(G).
\end{aligned} \tag{3}
$$

The following values

$$
\begin{aligned}
f(G) &= 9ab + 6a + 6b + 5, \\
n(G) &= 17(a+1)(b+1) + 6(4ab + 2a + 2b), \\
n_4(G) &= (a+1)(b+1), \\
m_{3,3}(G) &= 6ab + 3a + 3b,
\end{aligned}
$$

can be determined with no problem. Plugging them into (3) yields

$$
\begin{aligned}
M(Z(a,b); x, y) = 8(a+1)(b+1)x^2y^2 &+ 4(8ab + 5a + 5b + 2)x^2y^3 \\
&+ 3(2ab + a + b)x^3y^3 + 4(a+1)(b+1)x^3y^4.
\end{aligned}
$$

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