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Moments in graphs☆

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ABSTRACT

Let G be a connected graph with vertex set V and a *weight function* ρ that assigns a non-negative number to each of its vertices. Then, the ρ-*moment* of G at vertex u is defined to be $M_G^\rho(u) = \sum_{v\in V} \rho(v)\mathrm{dist}(u, v)$, where $\mathrm{dist}(\cdot, \cdot)$ stands for the distance function. Adding up all these numbers, we obtain the ρ-*moment of* G:

$$M_G^\rho = \sum_{u\in V} M_G^\rho(u) = \frac{1}{2}\sum_{u,v\in V} \mathrm{dist}(u, v)[\rho(u) + \rho(v)].$$

This parameter generalizes, or it is closely related to, some well-known graph invariants, such as the *Wiener index* $W(G)$, when $\rho(u) = 1/2$ for every $u \in V$, and the *degree distance* $D'(G)$, obtained when $\rho(u) = \delta(u)$, the degree of vertex u.

In this paper we derive some exact formulas for computing the ρ-moment of a graph obtained by a general operation called graft product, which can be seen as a generalization of the hierarchical product, in terms of the corresponding ρ-moments of its factors. As a consequence, we provide a method for obtaining nonisomorphic graphs with the same ρ-moment for every ρ (and hence with equal mean distance, Wiener index, degree distance, etc.). In the case when the factors are trees and/or cycles, techniques from linear algebra allow us to give formulas for the degree distance of their product.

1. Preliminaries

In general *graphs invariants* based on the distance between vertices (in chemistry, called *topological indices*) have found many applications in chemistry, since they give interesting correlations with physical, chemical and thermodynamic properties of molecules. Some well-known examples are the *Wiener index* $W(G)$ (introduced by Wiener [21]); the first and second *Zagreb indices* $M_i(G)$ (Gutman and Trinajstić [11], Zhou [24,25]), the *degree distance* (Dobrynin and Kotchetova [5] and Gutman [9]) and the *molecular topological index* $\mathrm{MTI}(G)$ (proposed by Schultz [16]).

Some results computing these indices for some graph operations (such as the Cartesian product, the join or the composition) and characterizing extremal cases have been given, among others, by Bucicovschi and Cioabă [3], Eliasi and Taeri [7], Khalifeh, Yousefi-Azari, Ashrafi, and Wagner [12,13], Tomescu [19], Tomescu [20], Yeh and Gutman [22], and Zhou [23,24]. In particular, Stevanović [18] computed the so-called Wiener polynomial of a graph, from which the Wiener and hyper-Winer [15] indices are retrieved. Moreover, it is worth mentioning that some of these indices are closely related. For instance, Klein, Mihalić, Plavšić, and Trinajstić [14] proved that, when G is a tree, there is a linear relation between $\mathrm{MTI}(G)$ and $W(G)$. (See also Gutman [9,10] for the study of other relations.)

As a generalization of most of the above indices, we define here the ρ-moment of a graph by giving some weights to its vertices. Then, we derive some exact formulas for computing the ρ-moment of a graph obtained by a general operation called

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'graft product', which can be seen as an extension of the hierarchical product [1], in terms of the corresponding ρ-moments of its factors. As a consequence, we provide a method for obtaining nonisomorphic graphs that have the same ρ-moment for every ρ. In the case when the factors are trees and/or cycles, algebraic techniques (distance matrices, eigenvalues, etc.) allow us to give formulas for the degree distance of their product. The remainder of this section is devoted to give some basic definitions and concepts on which our work relies.

1.1. Graphs and moments

Let G be a (simple and finite) connected graph with vertex set $V = V(G)$, $n = |V|$ vertices and consider a *weight function* $\rho : V \to [0, +\infty)$ that assigns a nonnegative number to each of its vertices. In particular, the *degree function* δ assigns to every vertex its degree. The *ρ-moment* of G at a given vertex u is defined as

$$M_G^\rho(u) = \sum_{v \in V} \rho(v)\mathrm{dist}(v, u),$$

where $\mathrm{dist}(\cdot, \cdot)$ stands for the *distance function*. Adding up all these numbers, we obtain the *ρ-moment of G*:

$$M_G^\rho = \sum_{u \in V} M_G^\rho(u) = \sum_{u \in V}\sum_{v \in V} \rho(v)\mathrm{dist}(v, u)$$

$$= \sum_{v \in V} \rho(v) \sum_{u \in V} \mathrm{dist}(v, u) = \frac{1}{2} \sum_{u,v \in V} \mathrm{dist}(u, v)[\rho(u) + \rho(v)].$$

This parameter generalizes, or it is closely related to, some well-known graph invariants, such as the following:

- The *mean distance* $d(G)$ of G is obtained when $\rho(u) = 1$ for each $u \in V$:

$$d(G) = \frac{1}{n^2} \sum_{u,v \in V} \mathrm{dist}(u, v) = \frac{1}{n^2} M_G^1.$$

- The *Wiener index* $W(G)$ [21] corresponds to the case $\rho(u) = 1/2$ for every $u \in V$:

$$W(G) = \frac{1}{2} \sum_{u,v \in V} \mathrm{dist}(u, v) = M_G^{1/2}.$$

- The *degree distance* $D'(G)$ proposed by Dobrynin and Kotchetova [5] (see also Gutman [9] where it was denoted $S(G)$, Tomescu [19], and Tomescu [20]) is obtained when $\rho(u) = \delta(u)$ for every $u \in V$, where δ stands for the *degree function*:

$$D'(G) = \frac{1}{2} \sum_{u,v \in V} \mathrm{dist}(u, v)[\delta(u) + \delta(v)] = M_G^\delta.$$

- The *Schultz index*, or *molecular topological index* $\mathrm{MTI}(G)$ [16], is obtained by adding up the first *Zagreb index* $M_1(G)$ [11], which is the sum of the squares of the degrees and the degree distance:

$$\mathrm{MTI}(G) = \sum_{u \in V} \delta(u)^2 + M_G^\delta.$$

1.2. The graft product

As commented, our aim here is to obtain some exact formulas for computing the ρ-moment of a graph, obtained by a 'general' operation, which is defined as follows: Given the connected graphs $H; K_1, \ldots, K_r$ with respective disjoint vertex sets $V_H; V_1, \ldots, V_r$ and some (root) vertices $x_i \in V_H$, $y_i \in V_i$, $i = 1, \ldots, r$, the *graft product*

$$G = H \begin{pmatrix} x_1 & \cdots & x_r \\ y_1 & \cdots & y_r \end{pmatrix} (K_1, \ldots, K_r) \quad (1)$$

is obtained by identifying vertices x_i and y_i for every $i = 1, \ldots, r$, as it is represented in Fig. 1.

Moreover, if $H; K_1, \ldots, K_r$ have weight functions $\alpha; \beta_1, \ldots, \beta_r$ respectively, we denote by $\gamma = \alpha + \beta_1 + \cdots + \beta_r$ the weight function of their graft product G defined as

$$\gamma = \begin{cases} \alpha(x) & \text{if } x \in H,\ x \neq x_i,\ 1 \le i \le r, \\ \alpha(x_i) + \beta_i(x_i) & \text{for } 1 \le i \le r, \\ \beta_i(y) & \text{if } y \in K_i,\ y \neq y_i,\ 1 \le i \le r. \end{cases}$$

In particular, when $r = 1$, the so-called *coalescence* $H \cdot K$ of the 'rooted graphs' (H, x) and (K, y) corresponds to the graft product $H \cdot K = H \binom{x}{y} K$, which has been studied in other contexts. For instance, Schwenk [17] related the characteristic polynomial of $H \cdot K$ in terms of the characteristic polynomials of H, $H - x$, K, and $K - y$. Namely,

$$\phi(H \cdot K) = \phi(H)\phi(K - y) + \phi(K)\phi(H - x) - x\phi(H - x)\phi(K - y).$$

Then, by applying iteratively this formula, we can calculate the characteristic polynomial of a (general) graft product.