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The Degree–Product Index of Narumi and Katayama

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Abstract

Let $G = (V, E)$ be a simple graph with vertex set V and edge set E ($|V| = n, |E| = m$), and let d_i be the degree of vertex i of G. The degree product $P(G) := \prod_{i=1}^{n} d_i$ of G was introduced and studied by Narumi and Katayama. This index is here fundamentally characterized; first, as the number of "functional" subgraphs of the directed graph $D(G)$ associated to G; and, second, as a suitable weighting over a certain class of ordinary subgraph covers of G. Then, $P(G)$ is related to several other common graph invariants by way of several bounding relations.

1 Introduction

Given a simple graph $G = (V, E)$ with vertex set V and edge set E, many different invariants have been considered. Two of the very simplest are $|V| = n$ and $|E| = m$. Others may be defined in terms of the vertex degrees, d_i ($1 \leq i \leq n$) for the ith vertex. One such simple topological index

$$P(G) := \prod_{i=1}^{n} d_i \tag{1}$$

was proposed, in 1984, by Narumi and Katayama [1, 2], as sharing a number of characteristics with the so-called Hosoya index [3], yet being much easier to compute. Along with the generally recognized chemical relevance of the Hosoya index $Z(G)$, this then motivated their study of the *degree product* $P(G)$. Later, $P(G)$ was further studied [4, 5] to find that it "gives back" the whole sequence of degrees, so long as the graph is connected and also so long as n and m are known and the degrees are ≤ 5, such as is the case for molecular graphs of saturated hydrocarbons. Some of this work [4] relates $P(G)$ for G a tree to certain weighted subgraph enumerations and to polynomials involving certain covers.

Here, we find that $P(G)$ counts so-called "functional" digraphs in the digraph $D(G)$ symmetrically derived from G, and we also find $P(G)$ to be a weighted evaluation of certain covers of G. Further, several inequalities are given to relate $P(G)$ to some other, better known graph invariants, such as the number $t(G)$ of all spanning trees of G. Also, in support of Narumi & Katayama's ideas [1, 2], we relate $P(G)$ to the Hosoya's index $Z(G)$ [3], which counts all matchings of G.

2 Preliminaries

We need first to recall certain terminology (see [6]) and results. A *digraph* (or *directed graph*) D is a graph each of whose edges is directed. If for each pair of vertices u and v of D, there exists a consistently oriented path from u to v, but not necessarily from v to u, then D is termed *weakly connected* (or *weak*). The *outdegree* (*indegree*) of a vertex v is the number of oriented lines (arcs and/or self-loops) that go out (come into) v, in D. In a *symmetric digraph*, an outdegree of each vertex v is equal to its indegree. In particular, one can obtain a symmetric digraph $D(G)$ from a simple graph G by the substitution of a pair of opposite arcs for each (undirected) edge of G.

A *functional digraph* is a digraph in which each vertex has outdegree one. Harary, Norman, and Cartwright (see p. 325 in [7] or p. 69 in [8]) demonstrated:

Proposition 1. *A digraph D is functional iff, first, each of its weak components consists of exactly one directed cycle Z (which may also be a self-loop or an edge), and, second, for each vertex u of Z, any weak component $R(u)$ of $D - Z$ which contains u is a tree oriented to the vertex u.*

That is, each weak component of functional digraph contains exactly one consistently oriented cycle (which, in general, may also be a self-loop or a pair of opposite arcs) while the other vertices, if any, belong to directed trees whose arcs are all oriented to the respective points of attachment to the cycle.

An entry a_{ij} of the adjacency matrix $A = [a_{ij}]_{i=1}^{n}$ of a simple (resp. functional) graph equals 1 iff the ith and jth vertices are adjacent (resp. there is an arc going from the ith vertex to the jth vertex); otherwise, $a_{ij} = 0$. The adjacency matrix $A[D(G)]$ of a derivative symmetric digraph $D(G)$ coincides with the adjacency matrix $A(G)$ of an original simple graph G, *i. e.*, $A[D(G)] = A(G)$.

A G-*cover* (or D-*cover*) is a subgraph whose vertex set is $V(G)$ (or $V(D)$). In this paper, we utilize the number $N_f(G)$ of all D-covers with components which are functional subgraphs. Also, we shall specially obtain the number $N_l(G)$ of all (weakly) connected functional subgraphs covering $D(G)$ which contain a pair of opposite arcs (also called a *fish*, or *lune*). Apparently, $N_l(G) \leq N_f(G)$, where the equality holds only for K_2 (since, by definition, G has no self-loops).

Besides another particular G-cover, we utilize several other graph structures. One such is that of a *tree*, which is an acyclic connected graph, and another is *bitree*, which is a graph with two components each of which is a tree. A tree or bitree, or indeed a general subgraph of G, is said to be *spanning* if this subgraph includes all the vertices of G. Yet another structure utilized is that of *matchings*, which are subsets of disjoint edges. And another is the "resistance distance" Ω_{ij} between 2 vertices i and j; this Ω_{ij} may be defined [9] as the effective electrical resistance between vertices i and j, when G is viewed as an electrical network with unit resistors on each edge. But also, there are [10] several other interpretations of Ω_{ij}, which further is a metric on G, and, then, may be used to generate different meaningful invariants. We make reference to several other graph invariants, which are introduced along the way.

Now, we turn to the derivation of our various results.

3 Equivalences

We begin this part with:

Proposition 2. *The symmetrical digraph $D(G)$ of a simple graph G has exactly $N_f(G) =$*

$\prod_{i=1}^{n} d_i = P(G)$ *covers which are functional subgraphs.*

Proof. By definition, the adjacency matrix of each functional subgraph has exactly one unit in every row. Thus, N_f equals the number of all simultaneous choices of n 1's, one from each of the rows of $A[D(G)]$. Since the ith $(1 \leq i \leq n)$ row contains exactly d_i 1's, a total number of such choices equals $\prod_{i=1}^{n} d_i = P(G)$, which is the proof. ■

Another auxiliary statement is:

Proposition 3. *Let $t(G)$ be the number of all spanning trees of an n-vertex graph G and let $N_l(G)$ be the number of all connected, spanning functional subgraphs, of $D(G)$, containing a lune. Then $t(G) = N_l(G)/(n-1)$.*

Proof. Apparently, each connected, spanning functional subgraph, of $D(G)$, containing a lune corresponds to a respective spanning tree of a graph G. In turn, to each spanning tree of G, there corresponds exactly $n-1$ such connected, spanning functional subgraphs of $D(G)$, where $n-1$ is the number of edges in a spanning tree of G. This correspondence produces the proof. ■

Now, we identify a correspondence to G-covers (of a certain type):

Proposition 4. *Let C be the set of all G-covers with components which are trees or connected subgraphs containing one cycle (of length ≥ 3). Then,*

$$P(G) = \sum_{\forall C \in \mathsf{C}} \prod_{\forall \gamma \in C} w_\gamma, \tag{2}$$

where w_γ is the weight of component γ of C, which is $w_\gamma = |V(\gamma)| - 1$ if γ is a tree and $w_\gamma = 2$ if γ contains a proper cycle of G.

Proof. First, note that the weight 2 of each unicyclic subgraph γ in C is due to the fact that this (undirected) cycle may receive two opposite orientations in a respective functional subgraph of $D(G)$, as described in Proposition 3. That is, this weight accounts for the two unicyclic graphs with opposite orientations of their 'common' cycle, in $D(G)$. The weight $|\gamma| - 1$, when γ is a tree, accounts for the different placements of lunes on it (as in Proposition 3). ■

This, in fact, is an example of a "family polynomial" (or F-polynomial, for short) of Farrell [11], whence relations generic for this family follow.

We might denote the part of $P(G)$ involving α tree components and β single-cycle-containing components by $P_{\alpha,\beta}(G)$. Then, for instance, Proposition 3 gives $P_{1,0}(G)$, and our next Proposition gives $P_{2,0}(G)$.

Proposition 5. *Let $W'(G) := \sum_{i<j} \Omega_{ij}$ be the resistance-distance sum, where Ω_{ij} is the resistance distance between vertices $i, j \in V(G)$, and let $t_2(G)$ be the number of spanning bitrees. Then, the spanning-bitree part of the sum of Proposition 4 is*

$$P_{2,0}(G) = t(G) \cdot W'(G) - (n-1)t_2(G). \tag{3}$$

Proof. It is known [12] that $\Omega_{ij} = t_{i,j}/t(G)$, where $t_{i,j}$ is the number of spanning bitrees $T_1 \oplus T_2$ with $i \in V(G)$ in one of components of $T_1 \oplus T_2$ and $j \in V(G)$ in the other component. Then,

$$W'(G) = (1/t(G)) \sum_{i<j} t_{i,j} = (1/t(G)) \sum_{T_1 \oplus T_2}^{\text{s.bitrees}} |V(T_1)||V(T_2)|,$$

where the sum $\sum_{T_1 \oplus T_2}$ ranges over all spanning bitrees of G; and $|V(T_1)||V(T_2)|$ is exactly the number of times which each bitree contributes to the sum $\sum_{i<j} t_{i,j}$, while considering all choices of vertices i in T_1 and j in T_2 (for T_1 and T_2 being an unordered pair of trees). Replacement of $|V(T_i)| = w_{T_i} + 1$ $(i = 1, 2)$, then, gives

$$W'(G) = (1/t(G)) \sum_{T_1 \oplus T_2}^{\text{s.bitrees}} (w_{T_1} w_{T_2} + w_{T_1} + w_{T_2} + 1).$$

But noting that $w_{T_1} + w_{T_2} = n - 2$, we obtain

$$t(G) \cdot W'(G) = \sum_{T_1 \oplus T_2}^{\text{s.bitrees}} w_{T_1 \oplus T_2} + (n-1)t_2(G).$$

Recognition of the spanning bitree sum here as the spanning bitree part $P_{2,0}(G)$ of the polynomial of Proposition 4, then, completes the proof. ■

4 Inequalities

Next, we proceed to several bounding relations:

Proposition 6. *Let $t(G)$ be the number of all spanning trees of a simple graph G. Then, $t(G) \leq (\prod_{i=1}^{n} d_i)/(n-1) = P(G)/(n-1)$, and equality holds iff G is a star.*

Proof. Our present desired inequality is due to the obvious one $N_l(G) \leq N_f(G)$ and Proposition 2. To obtain equality, there can be no contributions involving cyclic functional subdigraphs, where G must be acyclic. But to have only single-tree spanning functional subdigraphs, with each component having at least 2 vertices (corresponding to the lune) one must not be able to embed 2 disjoint edges in G, whence the longest path in G must be of length no more than 2, which, then, implies that G is a star. ■

We can add the following statement which uses more information about G:

Proposition 7. *Let $t(G)$ be the number of all spanning trees, and $\rho(G) = m - n + 1$ be the cyclomatic number of a graph G. Then,*

$$P(G) = N_f(G) \geq (n-1) \cdot t(G) + 2\rho(G). \tag{4}$$

Proof. Indeed, the family C of all functional subgraphs includes $(n-1) \cdot t(G)$ connected unicyclic subgraphs containing a lune and at least two covers containing each fundamental cycle of G (where this cycle has two opposite orientations). Since this inventory is not in general full, we easily arrive at the inequality obtained in (3). ■

This gives a (very slightly) better bound to $t(G)$ than Proposition 6.

When the number $\sigma(G)$ of all cycles in G is known, one may state a stronger analog of this last proposition, viz.:

Proposition 8. *Let $\sigma(G)$ be the number of all proper cycles of a graph G. Then,*

$$P(G) = N_f(G) \geq (n-1) \cdot t(G) + 2\sigma(G). \tag{5}$$

Proof. This follows similarly to the preceding two Propositions, now with a note that each cycle can be associated with at least one corresponding cycle-containing term γ in the expression of Proposition 4. ■

Proposition 9. *Let $W'(G)$ be the resistance sum, and let $t_2(G)$ be the number of all bitrees of a graph G. Then,*

$$P(G) \geq t(G) \cdot W'(G) + (n-1)[t(G) - t_2(G)]. \tag{6}$$

Proof. This follows from $P_{1,0}(G) + P_{2,0}(G) \leq P(G)$, along with Propositions 3 and 5. ■

In a similar vein, we can state the following:

Proposition 10. *Let $Z(G)$ be the total number of matchings, or Hosoya index, of G. Then,*

$$P(G) = N_f(G) \geq Z(G) - 1. \tag{7}$$

Proof. It is also similar to those of Propositions 6 and 7. Namely, to each of k-matchings, with $1 \leq k \leq \lfloor n/2 \rfloor$, of G, there corresponds at least one functional subgraph of $D(G)$, whereas the case $k = 0$, accounted by $Z(G)$, is rejected as a functional digraph. Hence, we arrive at the proof. ■

This result supports an observation [1] of Narumi and Katayama's that their index $(P(G))$ seems to be related to the Hosoya index $(Z(G))$; and, indeed, for a number of smaller trees, equality in our bound is found. However, a stronger correlation is found in the next statement which additionally involves values of $t(G)$ and m, viz.:

Proposition 11. *Let $Z(G)$ the number of all matchings of a graph G. Then,*

$$P(G) = N_f(G) \geq (n-1) \cdot t(G) + Z(G) - m - 1. \tag{8}$$

Proof. Apparently, $Z(G) - m - 1$ is the number of all matchings, of G, containing at least two edges, where we note that the empty graph is usually included as a matching in the count of $Z(G)$. Every such matching can be complemented to at least one forest of G with each component of the forest containing just one of the (≥ 2) edges of the matching. Since every forest of G corresponds to at least one cover C each of whose components contain a lune, we obtain, in general, an incomplete inventory of functional subgraphs (which also include $(n-1) \cdot T(G)$ monocomponent subgraphs containing one lune). Hence, the proof follows. ■

We can present here yet another result improving on the idea in Proposition 8:

Proposition 12. *Let $\mathrm{per}A(G)$ be the permanent of the adjacency matrix of a graph G with $|V(G)| \geq 3$, or, equivalently, of the symmetric digraph $D(G)$ (which, by definition, shares the same adjacency matrix with G). Then,*

$$P(G) = N_f(G) \geq (n-1) \cdot t(G) + \mathrm{per}A(G). \tag{9}$$

Proof. The family of all functional subgraphs of $D(G)$ includes also all covers of $D(G)$ with proper cycles. But $\mathrm{per}A$ counts the number of all covers with components which are either an edge (with weight 1) or a proper cycle, with weight 2. Together with $(n-1) \cdot t(G)$ connected spanning subgraphs containing one lune, these comprise, in general, not all functional subgraphs of $D(G)$, excepting any case where a contribution in $\mathrm{per}A(G)$ is such a spanning tree – as only occurs for the single edge graph with $|V(G)| = 2$. Hence, the proof is immediate. ■

Note that, for $|V(G)| = 2$, $D(G)$ contains only one lune and no proper cycle; thus, this case falls out of the conditions of Proposition 12.

Several of our bounds may be improved. For instance, the arguments to strengthen Proposition 6 to give Propositions 7 and 8 may be similarly applied to strengthen Proposition 9 to give:

Proposition 13. *Let $t(G)$ be the number of all spanning trees, and $\rho(G) = m - n + 1$ be the cyclomatic number of a graph G. Then,*

$$P(G) \geq t(G) \cdot W'(G) + (n-1)[t(G) - t_2(G)] + 2\rho(G). \tag{10}$$

And, similarly, we can state:

Proposition 14. *Let $\sigma(G)$ be the number of all proper cycles of a graph G. Then,*

$$P(G) \geq t(G) \cdot W'(G) + (n-1)[t(G) - t_2(G)] + 2\sigma(G). \tag{11}$$

Also, the arguments used to strengthen Proposition 6 to give Proposition 9 can be used to strengthen the inequalities of Propositions 11 and 12 to give:

Proposition 15. *Let $W'(G)$ be the resistance sum, and let $t_2(G)$ be the number of all bitrees of a graph G. Then,*

$$P(G) \geq t(G) \cdot W'(G) + (n-1)[t(G) - t_2(G)] + Z(G) - \mu(G;2) - m - 1, \tag{12}$$

where $\mu(G;2)$ is the number of matchings consisting of two disjoint edges.

And, similarly, another statement is:

Proposition 16. *Let $W'(G)$ be the resistance sum, and let $t_2(G)$ be the number of all bitrees of a graph G ($|V(G)| \geq 5$). Then,*

$$P(G) \geq t(G) \cdot W'(G) + (n-1)[t(G) - t_2(G)] + \mathrm{per}(G). \tag{13}$$

Though further relations might be possible involving tritrees and beyond to more profligate forests, we do not here attempt to consider such further invariants, as they are somewhat less commonly considered.

5 Discussion and conclusion

Besides the exact enumerations of Section 3, we have found several bounding relations in Section 4. One such in Proposition 6 bounds the number $t(G)$ of all spanning trees of a graph. This count $t(G)$ plays an important role in many applications of graph theory, so that several bounds for it have been proposed, as in [13] and bibl. In particular, Das [13] obtained the sharp upper bound $t(G) \leq [(2m - d_1 - 1)/(n-2)]^{n-2}$, where d_1 is the maximum vertex degree in G. Our bound $t(G) \leq P(G)/(n-1)$ is sometimes better than his. For instance, for a quadrangle, with $t(G) = 4$, Das' upper bound is $\lfloor [(2 \cdot 4 - 2 - 1)/2]^2 \rfloor = \lfloor (5/2)^2 \rfloor = 6$, while ours is $\lfloor (2 \cdot 2 \cdot 2 \cdot 2)/3 \rfloor = \lfloor 16/3 \rfloor = 5$. However, this situation is reversed for all cycles beginning from the 18-gon, for which $t(G) = 18$, Das' bound is $\lfloor [(2 \cdot 18 - 2 - 1)/16]^{16} \rfloor = 10722$, and ours is $\lfloor 2^{18}/17 \rfloor = 15420$. Indeed, both bounds render increasingly worse bounds for longer cycles, though both give sharp estimates for all stars, with $t(G) = 1$, and Das' bound is also sharp for all complete graphs, with $t(G) = 2^{n-2}$. It may be noted in general that most bounds, known for $t(G)$, are yet 'very approximate', and, indeed, ours of Proposition 6 is clearly expected to be very bad for larger graphs where many further terms ($P_{\alpha,\beta}(G)$ with $\alpha \neq 1$, $\beta \neq 0$) in the expansion of Proposition 4 are neglected. If $\rho(G)$ or $\sigma(G)$ are known, Propositions 7 and 8 yield modestly improved bounds on $t(G)$. The result of Proposition 10 yields a simple bound for the number $Z(G)$ of matchings, which, as we have already noted, achieves equality for a number of smaller tree graphs. Indeed, this bound for $Z(G)$ seems to us to be more generally better bound than that of Proposition 6 for $t(G)$. When other suitable invariants are known, then also Propositions 11 and 12 provide further bounds on $t(G)$. But in fact, Propositions 12 might be better used to give a bound on $\mathrm{per}A(G)$. Propositions 13–16 yield yet further bounding relations – though complicated by the numbers of invariants involved.

Indeed, our various boundary Propositions might be characterized in terms of which components in the expansion of Proposition 4 are treated. That is each boundary Proposition takes into account $P_{\alpha,\beta}(G)$ for selected values of α (the number of tree components) and β (the number of single-cycle-containing components):

Proposition	α, β
6	$1, 0$
7 & 8	$1, 0$ & $(0, \beta)$
9	$1, 0$ & $2, 0$
10	$(\alpha, 0)$
11	$1, 0$ & $(\alpha, 0), \alpha \geq 1$
12	$1, 0$ & $0, \beta$
13 & 14	$1, 0$ & $2, 0$ & $(0, \beta)$
15 & 16	$1, 0$ & $2, 0$ & $0, \beta$

Here, when an (α, β)-pair is enclosed in parentheses, the corresponding $P_{\alpha,\beta}(G)$ contribution is in general only approximated, whereas if not so parenthesized, it is dealt with exactly. Indeed, one might reexpress our various bonding propositions in terms of the $P_{\alpha,\beta}(G)$ (or certain sums on them) – but we do not pursue this here.

Next, we introduce two equivalent polynomials reflecting all the information contained in the degree sequence of a graph G, namely, $P^+(G;x) = \prod_{i=1}^{n}(x + d_i) = \sum_{s=0}^{n} a_s x^{n-s}$ and $P^-(G;x) = \prod_{i=1}^{n}(x - d_i) = \sum_{s=0}^{n}(-1)^s a_s x^{n-s}$. The former seems to be more convenient, while the latter has just vertex degrees $d_1, d_2, \ldots, d_n$ as its roots (but substitution of pluses for minuses, converts it into the former). One sees that $a_1 = 2m$ and $a_n = P^+(G;0) = (-1)^n P^-(G;0) = P(G)$, and yet further that, $a_2 = [4m^2 - M_1(G)]/2$, where $M_1(G) := \sum_{i=1}^{n} d_i$ is the first Zagreb index [14] (and also $a_2 = \mu(G,2) + \frac{1}{2}m(3m-1)$). Apparently, all a_i's are elementary symmetric functions of the degree sequence of G. By analogy with Proposition 2, it can be established:

Proposition 17. *A coefficient a_i $(0 \leq i \leq n)$ of x^{n-i}, in $P^+(G;x)$, equals the number of choices of i arcs (and/or self-loops) going out of exactly i vertices in $D(G)$.*

Proof. It elementarily follows from the definition of a (component of) functional digraph and uses arguments similar to those in the Proof of Proposition 2. ■

That is, the case of Proposition 17 deals with all i-arc covers which, along with unicyclic digraphs, may also contain, for $i < n$, directed subtrees whose arcs are oriented, in each subtree, to one of vertices. Taking into account the ease of calculation of a_i's, it is very interesting to find also different interpretations of these numbers, especially those which may be utilized in practice. Therefore, we just pose here a problem about the combinatorial nature of all coefficients of $P^{+}(G;x)$, which is also addressed to the reader.

In conclusion, we have obtained new alternative representations of the degree product $P(G)$, first, as a functional-digraph enumerator, and, second, as a weighted enumerator of certain G-covers. These both are "family polynomials" (or F-polynomials, for short), for which, then, further relations follow, as explicated by Farrell [11]. And further, we have found that $P(G)$ is related to a diversity of other graph invariants. And yet further, we have introduced a novel new invariant $P^{\pm}(G;x)$, which is related to the degree product $P(G)$ much as the matching polynomial is related to Hosoya's [3] matching number $Z(G)$. An inference (following from our Proposition 10) supports an observation [1] of Narumi and Katayama that their index $(P(G))$ seems to be related to the Hosoya index, and further our degree-product polynomials $P^{\pm}(G;x)$ may be viewed as analogs of the matching polynomial. We have also found relations to a variety of other graph invariants (including the resistance-distance Wiener sum and the permanent of A). The results here suggest a fundamental nature for $P(G)$.

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