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A Note on the Parity of Integer-Valued Topological Indices

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Abstract

In this note we collect and state some facts on the parity of some integer-valued graph invariants. In particular, we show that several well-known bond-additive topological indices assume only even values for all connected graphs. Among them are both degree-based and distance-based indices. We also discuss some general graph-theoretical consequences of established results.

1 Introduction

One of the first results learned by any aspiring student of graph theory is the celebrated *Handshaking lemma*, stating that in any graph, the number of vertices of odd degree must be even. It follows at a glance, by observing that the sum of all degrees is equal twice the number of edges, and hence even. In this note we show how the same idea can be used to establish the parity of several other integer-valued graph invariants. Our results could be useful in studying inverse, or realizability problems for integer-valued topological indices.

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2 Integer-valued degree-based bond-additive invariants

All graphs in this paper are simple and connected. In particular, they do not have isolated vertices. For a graph G, we denote its vertex set by $V(G)$, and its edge set by $E(G)$. If an edge e has the vertices u and v as its end-vertices, we write $e = uv$.

A *topological index* $I(G)$ is any numerical quantity related to the structure of a graph G which does not depend on labeling of its vertices. A topological index $B(G)$ is *bond-additive* if it is defined as

$$B(G) = \sum_{e \in E(G)} \varphi(e),$$

where $\varphi(e)$ is the *contribution* of the edge e. If the contribution φ is defined in terms of degrees of the end-vertices of $e = uv$, i.e., if $\varphi(e) = \varphi(d_u, d_v)$, then $B(G)$ is a degree-based bond-additive invariant of G.

If $B(G)$ has integer values, it makes sense to consider their parity. Clearly, integrality of $B(G)$ will follow if the contributions $\varphi(d_u, d_v)$ are themselves integral. (The opposite is not necessarily true.) Hence, we should determine how the parities of contributions affect the overall parity of $B(G)$. To this end, we define the function $\pi : \mathbb{N} \to \mathbb{N}$ as the remainder of division of n by 2. Hence, $\pi(n) = 0$ for n even, and $\pi(n) = 1$ for n odd. It will allow us to concisely state our main results in the following section.

3 Main results

Theorem 1. *Let $B(G)$ be an integral degree-based bond-additive invariant with edge contributions $\varphi(d_u, d_v)$. If*

$$\pi(\varphi(x, y)) = \pi(x + y)$$

for all $x, y \in \mathbb{N}$, then $B(G)$ is even for any connected graph G.

Proof. By the Handshaking lemma, the number of vertices of odd degree in G must be even. But then the first Zagreb index of G,

$$M_1(G) = \sum_{u \in V(G)} d_u^2,$$

must be even. As observed in [7], the first Zagreb index can be expressed in terms of edge contributions,

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

Hence the number of odd contributions $d_u + d_v$ must be even. Now, the condition $\pi(\varphi(x, y)) = \pi(x + y)$ implies that the number of odd contributions to $B(G)$ must be even, and hence, $B(G)$ itself must be even. ■

4 Consequences

Now we list several consequences of our main result. Some of the obtained results have been known, but some seem to be new. We start with listing some topological indices which must have even values for all connected graphs. A convenient list of degree-based bond-additive indices, together with their defining contributions, can be found in [4]. For the integer-valued ones among them, we have the following result.

Corollary 1. *Let G be a connected graph. Then the following bond-additive topological indices of G must have even values:*

- *first Zagreb index,* $\varphi(x, y) = x + y$;
- *forgotten index,* $\varphi(x, y) = x^2 + y^2$;
- *Platt index,* $\varphi(x, y) = x + y - 2$;
- *hyper-Zagreb index,* $\varphi(x, y) = (x + y)^2$;
- *Albertson irregularity,* $\varphi(x, y) = |x - y|$;
- *sigma irregularity,* $\varphi(x, y) = (x - y)^2$;
- *redefined 3. Zagreb index,* $\varphi(x, y) = xy(x + y)$;

- *2. hyper-Gourava index,* $\varphi(x,y) = (xy(x+y))^2$.

Proof. For the first six listed indices, the claim follows by verifying that their edge contributions satisfy the conditions of Theorem 1. For the remaining two indices, note that their contributions are always even. ■

The list of indices in Corollary 1 is not exhaustive. It can be extended by including several general(ized) indices for special, most often integral, values of generalizing parameters.

Corollary 2. *Let G be a connected graph. Then the following topological indices of G have even values for all positive integer values of α:*

- *the general first Zagreb index* $M_1^\alpha(G) = \sum_{u \in V(G)} d_u^\alpha$*;*
- *the general sum-connectivity index* $\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha$*;*
- *the generalized complementary 2. Zagreb index* $cM_\alpha(G) = \sum_{uv \in E(G)} \left| d_G(u)^\alpha - d_G(v)^\alpha \right|$.

The list of indices in Corollary 2 is also non-exhaustive. We invite the reader to extend it to other sub-classes of generalized indices.

As the last result in this section, we look at the first Zagreb coindex. We refer the reader to [3, 6] for definition of Zagreb coindices and motivations for their study.

Corollary 3. *Let G be a connected graph. Then the first Zagreb coindex $\overline{M}_1(G)$ is even.*

Proof. It has been observed in [7] that $M_1(G) + \overline{M}_1(G) = 2m(n-1)$, where n and m denote the number of vertices and the number of edges of G, respectively. The result now follows from the even parity of $M_1(G)$. ■

5 Digression – distance-based indices

We now make a digression toward distance based indices and revisit several less known facts about their parity. Here we cannot use Theorem 1, but we can still rely on the Handshaking lemma. We start by establishing a Handshaking lemma-type result for vertex transmissions.

The *transmission* $Tr(u)$ of a vertex $u \in V(G)$ is the sum of all (shortest-path) distances from u to all other vertices of G,

$$Tr(u) = \sum_{v \in V(G)} d(u,v).$$

The *Wiener index* $W(G)$ of a connected graph G is nowadays usually defined as the sum of all pairwise distances in G, but it started its career in [11] as a bond-additive index, defined for trees as $W(T) = \sum_{uv \in E(T)} \varphi(e)$, with the contribution of e defined as the number of shortest paths between vertices of T passing through e. The two definitions are equivalent for trees, but not for general graphs.

Proposition 2. *In every connected graph G, the number of vertices with odd transmission is even.*

Proof. The sum of all transmissions in G is equal to twice the Wiener number of G, hence even. Then the number of vertices with odd transmissions must be even. ■

The Wiener index itself can have both even and odd values. In some cases, however, we may specify its parity.

Proposition 3. *Let T_n be a tree with an odd number of vertices. Then $W(T_n)$ is even.*

Proof. According to the original definition of the Wiener index for trees,

$$W(T_n) = \sum_{uv \in E(T_n)} n_u n_v.$$

(Here n_u denotes the number of vertices in T_n closer to u than to v; n_v is defined analogously.) Since $n = n_u + n_v$ is odd, one of n_u and n_v must be even, and all contributions are even. ■

The above result has been observed several times so far [5,10]. It would be interesting to investigate what is the largest power of two dividing $W(T_n)$ for different types of odd trees.

Next, we look at the Mostar index. It is a recently introduced index [8] defined as

$$Mo(G) = \sum_{uv \in E(G)} |n_u - n_v|.$$

We refer the reader to a recent review [1] for more on its properties and uses. Its possible values for various graph classes and the inverse problem were recently studied in [2, 9]. We state here a parity result implicitly present, but not proved in [9].

Proposition 4. *Mostar index of any tree is an even integer.*

Proof. For a tree on an even number of vertices, n_u and n_v are of the same parity for each edge. So, their differences, i.e., the edge contributions, are all even and the sum is even.

If the number of vertices is odd, all contributions are odd, but their number is even, so the sum is again even. ∎

We invite the reader to investigate for which other classes of graphs one can obtain analogous results.

6 Coda

We close this note by a general graph theoretical result which does not seem to be explicitly stated in the literature.

Theorem 5. *Let G be a connected graph. Then the number of edges connecting vertices whose degrees are of the opposite parity is even.*

Proof. The claim follows directly from Theorem 1 and the even parity of $M_1(G)$. ∎

Besides being of general graph-theoretical interest, the above observation might be useful and interesting in the context of chemical graphs, which have a small number of possible degrees and hence a small number of different edge types. Hence, the standard way of computing many degree-based indices of chemical graphs is by multiplying contributions $\varphi(i, j)$ by the number of edges m_{ij} connecting vertices of degree i and j

and then summing over all edge types. Our result implies that, for any chemical graph, m_{12}, m_{14}, m_{23} and m_{34} are all even.

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