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On topological indices of certain interconnection networks ☆

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ABSTRACT

In QSAR/QSPR study, physico-chemical properties and topological indices such as Randić, atom-bond connectivity (*ABC*) and geometric-arithmetic (*GA*) index are used to predict the bioactivity of chemical compounds. A topological index is actually designed by transforming a chemical structure into a numeric number. These topological indices correlate certain physico-chemical properties like boiling point, stability, strain energy etc of chemical compounds. Graph theory has found a considerable use in this area of research.

The topological properties of certain networks are studied recently in [13] by Hayat and Imran (2014). In this paper, we extend this study to interconnection networks and derive analytical closed results of general Randić index $R_\alpha(G)$ for different values of "α" for butterfly and Benes networks. We also compute first Zagreb, *ABC*, and *GA* indices for these important classes of networks. Moreover, we construct two new classes of mesh derived networks by using some basic operations of graphs on $m \times n$ mesh networks, and then study certain topological indices for these classes of networks.

1. Introduction and preliminary results

Cheminformatics is new subject which is a combination of chemistry, mathematics and information science. It studies Quantitative structure–activity (QSAR) and structure–property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds. In the QSAR/QSPR study, physico-chemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index and *ABC* index are used to predict bioactivity of the chemical compounds.

A *topological index* is a function "*Top*" from '$\sum$' to the set of real numbers, where '$\sum$' is the set of finite simple graphs with property that $Top(G) = Top(H)$ if both G and H are isomorphic. There is a lot of research which has been done on topological indices of different graph families so far, and is of much importance due to their chemical significance. A topological index is actually a numeric quantity associated with chemical constitution purporting for correlation of chemical structure with many physico-chemical properties, chemical reactivity or you can say that biological activity. Actually topological indices are designed on the ground of transformation of a molecular graph into a number which characterize the topology of that graph.

Butterfly graphs are defined as the underlying graphs of Fast Fourier Transforms (FFT) networks which can perform the FFT very efficiently. The butterfly network consists of a series of switch stages and interconnection patterns, which allows 'n' inputs to be connected to 'n' outputs. The *Benes network* consists of back-to-back butterflies. As butterfly is known for FFT, Benes is known for permutation routing [2]. The butterfly and Benes networks are important multistage interconnection

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networks, which possess attractive topologies for communication networks [20]. They have been used in parallel computing systems such as IBM, SP1/ SP2, MIT Transit Project, NEC Cenju-3 and used as well in the internal structures of optical couplers [19,31]. The multistage networks have long been used as communication networks for parallel computing [17].

Multiprocessor interconnection networks are often required to connect thousands of homogeneously replicated processor-memory pairs, each of which is called a processing node. Instead of using a shared memory, all synchronization and communication between processing nodes for program execution is often done via message passing. Design and use of multiprocessor interconnection networks have recently drawn considerable attention due to the availability of inexpensive, powerful microprocessors and memory chips [5]. The mesh networks have been recognized as versatile interconnection networks for massively parallel computing. This is mainly due to the fact that these families of networks have topologies which reflect the communication pattern of a wide variety of natural problems. Mesh/torus-like low-dimensional networks have recently received a lot of attention for their better scalability to larger networks, as opposed to more complex networks such as hypercubes [6]. There is a lot of relevant works on interdependent networks which can be reviewed. In particular the failure of cooperation on dependent networks has been studied a lot recently in [16,21,27–29]. For literature review of related topics please see [21–23].

A graph $G(V, E)$ with vertex set V and edge set E is connected, if there exist a connection between any pair of vertices in G. A *network* is simply a connected graph having no multiple edges and loops. A *chemical graph* is a graph whose vertices denote atoms and edges denote bonds between that atoms of any underlying chemical structure. The *degree* of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph the degree of any vertex is at most 4. The *distance* between two vertices u and v is denoted as $d(u, v) = d_G(u, v)$ and is the length of shortest path between u and v in graph G. The length of shortest path between u and v is also called $u - v$ *geodesic*. The longest path between any two vertices is called $u - v$ detour.

In this article, G is considered to be network with vertex set $V(G)$ and edge set $E(G)$, d_u is the degree of vertex $u \in V(G)$ and $S_u = \sum_{v \in N_G(u)} d(v)$ where $N_G(u) = \{v \in V(G) | uv \in E(G)\}$. The notations used in this article are mainly taken from books [7,9].

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin. He named this index as *path number*. Later on, path number was renamed as *Wiener* index [30] and then theory of topological index started.

Definition 1.0.1. Let G be a graph. Then the Wiener index of G is defined as

$$W(G) = \frac{1}{2}\sum_{(u,v)} d(u, v),$$

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is $u - v$ geodesic.

The very first and oldest degree based topological index is *Randić* index [24] denoted by $R_{-\frac{1}{2}}(G)$ and introduced by Milan Randić in 1975.

Definition 1.0.2. The Randić index of graph G is defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The general Randić index was proposed by Bollobás and Erdös [3] and Amic et al. [1] independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists [14]. Many important mathematical properties have been established [4]. For a survey of results, we refer to the new book by Li and Gutman [18].

The general Randić index $R_\alpha(G)$ is the sum of $(d_u d_v)^\alpha$ over all edges $e = uv \in E(G)$ defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha.$$

Obviously $R_{-\frac{1}{2}}(G)$ is the particular case of $R_\alpha(G)$ when $\alpha = -\frac{1}{2}$.

An important topological index introduced about forty years ago by Ivan Gutman and Trinajstić is the *Zagreb* index or more precisely first zagreb index denoted by $M_1(G)$ and was defined as the sum of degrees of end vertices of all edges of G.

Definition 1.0.3. Consider a graph G, then first zagreb index is defined as

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

The second Zagreb index is defined in the following way.

Definition 1.0.4. Consider a graph G, then second zagreb index is defined as