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# ABSTRACT

The complementary prism of G, denoted by  $G\overline{G}$ , is the graph obtained from the disjoint union of G and  $\overline{G}$  by adding edges between the corresponding vertices of G and  $\overline{G}$ . Up to date, the progress of experimental research around complementary prisms is limited by the unavailability of publicly available instances that could be used to run extensive experiments and to compare the performance on different topological index solutions and its bounds. For this reason, we decided to make publicly available 435 instances of type  $G\bar{G}$ randomly generated, with increasing network size (from 12 to 1948 nodes). The dataset presents instances of Complementary Prism Networks suitable to measure the Wiener Index and Generalized Wiener Index and the value of these indices for these instances. In addition, are presented the value of some lower and upper bounds proposed in the literature for these indices and their error with respect to the value of the index.

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#### Specifications Table

Subject	Discrete mathematics and combinatorics
Specific subject area	The dataset presents instances of Complementary Prism Networks, the value of the Generalized Wiener Index, some lower and upper bounds of these indices for these instances.
Type of data	Table Graph Instances
How the data were acquired	Each instance was generated randomly using the language $C++$ (Microsoft Visual Studio) on a personal computer with Intel Core i7-9750H (2.6 GHz) and 16 GB of RAM DDR4. We implemented the Wiener Index, Generalized Wiener Index, some lower and upper bounds of these indices using the language $C++$ .
Data format	Raw Analyzed
Description of data collection	We generated the instances using different pseudo-random methods to generate the graphs $G$ of $G\tilde{G}$ . The order and the size of each $G$ was generated randomly using function $rand()$ within the respective ranges. Each new edge was added in between two yet non-adjacent vertices randomly until the corresponding size was attained.
Data source location	Acapulco de Juárez, Guerrero, México.
Data accessibility	Repository name: Mendeley Data
	Data identification number: 10.17632/3cz2dj3hzz.3
Deleted we even h	Direct URL to data: https://data.mendeley.com/datasets/3cz2dj3hzz/3
article	J. menaez, K. keyes, J. M. koanguez, J. M. Sigarreta, Geometric and topological properties of the complementary prism networks, Math Meth Appl Sci. 46 (2023) 9555-9575. https://doi.org/10.1002/mma.9074

## 1. Value of the Data

- The dataset offers different topological structures of networks that researchers in the fields of Graph Theory and topological indices can utilize as test instances and benchmarks for evaluating and comparing topological indices.
- The network topologies and parameters provide in this work can be used for the performance evaluation of lower and upper bounds proposed in the literature for the Wiener Index and Generalized Wiener Index [1,2].
- The dataset serves as a basis to generate new datasets, such as generalized complementary prisms [3], and experimentally evaluated their topological, metric, and/or structural properties.
- The dataset contains a random graphs sub-dataset *G* and its complementary operator  $\overline{G}$ , which has been extensively studied in a theoretical way [4,5]. This dataset will allow the development of your experimental studies.

# 2. Objective

Up to date, the progress of experimental research around complementary prisms is limited by the unavailability of publicly available instances that could be used to run extensive experiments and to compare the performance of different topological index solutions and their bounds. The goal of this work is to provide network topologies (complementary prisms) that can be used as test instances and benchmarks for evaluating and comparing topological indices.

## 3. Data Description

The dataset includes 435 instances of Complementary Prism Networks [1] and the corresponding reference parameters for the networks. Random topologies are provided, with increasing network size (from 12 to 1948 nodes). The structural information of the networks is sum-



Fig. 1. Example random complementary prism networks: (a)  $G\bar{G}$ , (b)  $G\bar{G}$  instance structure.

marized and exemplified in Fig. 1b, which reports the numbers of nodes, edges, and adjacency matrix of the network.

All instances are publicly available in the Mendeley Data repository [6]. In the repository, the instances are provided in the folder *BD\_GGc*. The folder contains 435 text files of the topology data of the instances stored (see Fig. 1b).

The Excel workbook *Experimentos\_GGc.xlsx* contains two spreadsheets (*Exp\_GGc* and *Graph*). The spreadsheet *Exp\_GGc* aims to collect and summarize the value of the Wiener Index, Generalized Wiener Index [2], and some lower and upper bounds proposed in [1] for these indices and their percentage error [1] for the instances available in the dataset [6]. The spreadsheet *Graph* summarizes graphically, in six graphs, the results that were collected in spreadsheet *Exp\_GGc*.

#### 4. Experimental Design, Materials, and Methods

The complement of a graph *G* is a graph  $\overline{G}$  on the same vertices such that two distinct vertices of  $\overline{G}$  are adjacent if and only if they are not adjacent in *G*. That is, to generate the complement of a graph, one fills in all the missing edges required to form a complete graph and removes all the edges that were previously there [5]. We would like to point out that the complementary prism of G = (V, E), denoted by  $G\overline{G}$ , is the graph obtained from the disjoint union of *G* and  $\overline{G}$  by adding edges between the corresponding vertices of *G* and  $\overline{G}$  [1]. For example, the Petersen graph is a complementary prism, such that  $G = C_5$  (see Fig. 2).

# 4.1. Method for GG generation

We describe hereafter the process we followed to generate the instances of Complementary Prism Networks ( $G\bar{G}$ ), starting from randoms graph *G*. Each instance of  $G\bar{G}$  is built in two stages. In the first stage, a random graph *G* is generated. In the second stage, the adjacency matrix of  $G\bar{G}$  is constructed using the adjacency matrices of *G* and  $\bar{G}$ .

In the first stage, each graph *G* was generated randomly using the language C++ (Microsoft Visual Studio) in a personal computer with Intel Core i7-9750H and 12 GB of RAM DDR4. The order and the size of *G* was generated randomly using function *rand*() within the respective ranges (11 < |V(G)| < 1000 and density of *G* between 0.2 and 0.7). In C++ the function *rand*() is defined in header file <cstdlib>. This is used to generate a random number in the range [0, *RAND\_MAX*). The random number is generated by using an algorithm that gives a series of



**Fig. 2.** Complementary prism  $C_5\overline{C_5}$  (Modified from [1]).



Fig. 3. Structure adjacency matrix of GG.

non-related numbers whenever this function is called. *RAND\_MAX* it is a constant whose default value may vary between implementations, in our case  $RAND_MAX_1 = 1000$  and  $RAND_MAX_2 = 5000$ . This function does not take any parameters.

On the other hand, graph density represents the ratio between the edges present in a graph and the maximum number of edges that the graph can contain. It's particularly useful when we have a graph and want to add new edges to the graph. Moreover, graph density gives us an idea of how many edges we can still add to the network. Now, derived the formula for graph density.

$$density(G) = \frac{2|E(G)|}{|V(G)|(|V(G)| - 1)}.$$

Let n = |V(G)|, to ensure that *G* is a connected graph, the first n - 1 edges were inserted as follows. For all  $x_i \in V(G)$ , if  $i \ge 2$ , the edge  $(x_j, x_i)$  is uncertain such that j < i and j is randomly selected. Each new edge was added in between two yet non-adjacent vertices randomly until the corresponding density was attained.

In the second stage, the Complementary Prism Networks  $(G\overline{G})$  is constructed from the random graph G. Let M and  $\overline{M}$  be the adjacency matrices of G and  $\overline{G}$  respectively. The adjacency

# **Algorithm 1** Generation $G\overline{G}$

```
Input: RAND_MAX_1 and RAND_MAX_2.
Output: Adjacency matrix of G\overline{G}.
n \leftarrow \text{random number between 10 and } RAND_MAX_1;
                                                                            \triangleright This is |V(G)|
d \leftarrow random number between 0.2 and RAND_MAX_2/10000;
                                                                            \triangleright This is |E(G)|
m \leftarrow |d * n(n-1)/2|;
M \leftarrow matrix of n rows and n columns initialized to zero;
M[1][2] \leftarrow 1;
M[2][1] \leftarrow 1;
for i = 3 : n do
    j \leftarrow random number between 1 and i - 1;
    M[j][i] \leftarrow 1;
    M[i][j] \leftarrow 1;
end for
h \leftarrow n - 1;
while h \leq m do
    x \leftarrow random number between 1 and n;
    y \leftarrow random number between 1 and n;
    if x \neq y and M[x][y] \neq 1 then
        M[x][y] \leftarrow 1;
        M[y][x] \leftarrow 1;
        h \leftarrow h + 1:
    end if
end while
I \leftarrow \text{identity matrix of order } n;
\overline{M} \leftarrow matrix of n rows and n columns initialized to zero;
for i = 1 : n do
    for j = i + 1 : n do
        if M[i][j] \neq 1 then
            M[i][j] \leftarrow 1;
             \overline{M}[j][i] \leftarrow 1;
        end if
    end for
end for
M\overline{M} \leftarrow concatenate the matrices M, I, and \overline{M}, as shown in Figure 3;
```

return  $M\overline{M}$ ;

Fig. 4. Method for GG generation.

matrix of  $G\bar{G}$  is constructed following the structure shown in Fig. 3, where  $I_n$  is the identity matrix of order n. Note that  $|V(G\bar{G})| = 2n$  and  $I_n$  are the edges between the corresponding vertices of G and  $\bar{G}$ .

Below we give a formal description of the method (Fig. 4).

# 4.2. Wiener index and generalized Wiener index

The Wiener Index, the Generalized Wiener Index, and the lower and upper bounds studied [1] were programmed in C++. The Wiener index of *G* is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

where  $\{u, v\}$  runs over every pair of vertices in *G*. On the other hand, the Generalized Wiener Index is defined in the following way:

$$W^{\lambda}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)^{\lambda},$$

with  $\lambda \in \mathbb{R}$ . The experiments were performed on the same computer as mentioned above. By the definition of the Wiener Index and the Generalized Wiener Index, it is required to calculate the minimum distance (d(u, v)) between every pair of vertices in the network. The Dijkstra algorithm was used for this purpose. Dijkstra's algorithm is an algorithm for determining the shortest path, given an origin vertex, to the rest of the vertices in a graph that has weights on each edge. In our case, each edge has a weight equal to one. The idea of this algorithm consists of exploring all the shortest paths starting from the source vertex and leading to all the other vertices; when the shortest path from the source vertex to the rest of the vertices that make up the graph is obtained, the algorithm stops [7].

#### **Ethics Statements**

Not applicable. This work does not contain any studies with human or animal subjects.

#### **Data Availability**

Complementary Prism Networks (Original data) (Mendeley Data).

## **CRediT Author Statement**

**Ernesto Parra-Inza:** Conceptualization, Methodology, Software, Data curation, Writing – original draft, Visualization; **José María Sigarreta-Almira:** Conceptualization, Methodology, Validation, Writing – review & editing, Formal analysis.

#### **Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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