

# Efficient computation of the Wiener Index for a class of planar graphs

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## Abstract

WRITTEN LAST. Computation of the Wiener Index for a graph on  $n$  vertices, using the definition, is of order  $n^2$ . We give an algorithm that applies to a certain class of planar graphs, which is of smaller order.

## 1 Introduction

The Wiener Index is an important metric in chemical graph theory as it closely correlates with the boilings points of alkane molecules, along with many other parameters of the molecule, such as density, surface tension and viscosity of its liquid phase [5]. Direct computation of the Wiener index from the definition, for a graph with  $n$  vertices, is of the order  $O(nm)$ , where  $n$  is the number of vertices and  $m$  is the number of edges in the graph. It is of practical and theoretical interest to find a more efficient algorithm for computing the Wiener index.

We consider a certain class of planar graphs, called partial cubes, the definition is well known, see for example [3], but will be reviewed in section 2. In section 3 we introduce an algorithm using cut methods to calculate the Wiener Index in linear time for this class of graphs.

## 2 Definitions

Before we talk about the algorithm, we need to introduce and recall some definitions. We need to talk about the class of graphs we are working with, and some terms used.

Of course, the most important thing to introduce is the Wiener Index itself. In 1971, Hosoya extended the original definition of the Wiener Index from trees to all connected Graphs  $G$  by the following definition[1].

**Definition 1.** The Wiener Index of a graph,  $G$ , is given by

$$W(G) = \sum_{\{u,v\} \in V(G)} d_G(u,v).$$

**Definition 2.** [3] Let  $G$  be a connected graph, then  $G$  is a **partial cube** if its vertices  $u$  can be labeled with binary strings  $l(u)$  of a fixed length, such that

$$d_G(u,v) = H(l(u), l(v))$$

holds for any vertices  $u$  and  $v$  of  $G$ , where  $H(l(u), l(v))$  is the Hamming distance of the binary strings  $l(u)$  and  $l(v)$ .

This is the class of graphs we will be talking about for the rest of this paper.

We now need to introduce an *elementary cut*, which is a key component of the algorithm.

**Definition 3.** Let  $G = (V, E)$  be a simple connected planar graph, all of whose cycles are of even length, which we assume to be embedded in the plane. An **elementary cut** is a sequence

$$e_1 F_1 e_2 F_2 \cdots e_k F_k e_{k+1}$$

such that

- Each  $e_i$  is an edge in the graph
- Each  $F_i$  is a face in the graph
- Edges  $e_i$  and  $e_{i+1}$  are antipodal edges belonging to the face  $F_i$
- The first and last edges  $e_1$  and  $e_{k+1}$  lie on the boundary of the embedding.

It is a well known result (see [3]) that the Wiener index can be calculated on partial cubes by the following theorem.

**Theorem 1.** Let  $G$  be a partial cube and  $C_i$  be an elementary cut. Let  $n_1(C_i)$  and  $n_2(C_i)$  be the number of vertices in the two connected components of  $G - C_i$ , that is, the graph created by taking the elementary cut  $C_i$ . Then

$$W(G) = \sum_{i=1}^k n_1(C_i) n_2(C_i).$$

Cut methods have been used in the past to calculate the Wiener index of chemical graphs [2]. We present a faster way to calculate the weiner index on a partial cube.

### 3 The Algorithm

The algorithm can be separated into two main components.

1. Find the elementary cuts;
2. Count the number of vertices on either side of all the cuts.

The first of these can be achieved by algorithm 1.

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**Algorithm 1** Elementary Cut Finding Algorithm

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1: for all edges in  $G$  do
2:   Join the edge to it's adjacent face.
3:   Increment a counter on the face by one, to keep track of the size of
   each cycle.
4: end for
5: for all boundary edges do
6:   Create a cut by tracing the unique path from edge to face to the
   antipodal edge, until another boundary edge is reached.
7: end for
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The second of these can be achieved by algorithm 2.

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**Algorithm 2** Counting Vertices

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1: for a do
2:   b
3: end for
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### 4 Proof(s)

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### References

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