THE LATTICE DIMENSION OF BENZENOID SYSTEMS

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Abstract

A labeling of vertices of a benzenoid system B is proposed that reflects the graph distance in B and is significantly shorter that the labeling obtained from a hypercube embedding of B. The new labeling corresponds to an embedding of B into the integer lattice $\mathbb{Z}^d$ and is shown to be optimal for all practical purposes. A coordinatization algorithm is presented and it is demonstrated that it can be easily carried out by hand.

Key words: Benzenoid system; Lattice dimension; Isometric dimension; Algorithm

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1 Introduction

Benzenoid systems (molecular graphs of benzenoid hydrocarbons) are one of the most studied classes of graphs within the chemical graph theory, we refer to the books [6, 12] dedicated to these systems and a sample of papers on different aspects of these graphs [7, 9, 10, 14, 21–29]. It is therefore not surprising that many names have been given to benzenoid systems, notably hexagonal systems. (For the list of all names see [10].)

One of the important features of benzenoid systems is that they can be isometrically embedded into hypercubes, the fact first observed in [18]. This observation led to many investigations of benzenoid systems [2, 4, 5, 15, 19], to investigations of other chemical graphs that can also be isometrically embedded into hypercubes, for instance of phenylenes, see [13], and to more general embeddings of (chemical) graphs [3].

It clearly turned out that an isometric embedding of a benzenoid system into a hypercube has many advantages. There is, however, one drawback of this approach. The number of coordinates of an embedding of a benzenoid system B into a hypercube is equal to the number of the elementary cuts of B. Therefore, if B is not very small, the vertex labels become large. Hence for bigger benzenoid systems the investigations are not easily carried out "by hand". In this paper we propose another labeling of benzenoid systems that also reflects the vertex distance but is significantly shorter that the labeling obtained from the isometric hypercube embedding. To be more precise, we label vertices u of a benzenoid system B with labels

$$\ell(u) = (\ell_1(u), \ell_2(u), \ldots, \ell_d(u)), \quad \ell_1(u), \ldots, \ell_d(u) \in \mathbb{Z}\,,$$

such that

$$d_B(u,v) = \sum_{i=1}^{d} |\ell_i(u) - \ell_i(v)|\,,$$

where $d_B(u,v)$ is the usual shortest path distance in B. Such embeddings of graphs into $\mathbb{Z}^d$ are called *lattice embeddings*. The minimum possible d for which there exists a lattice embedding of B is called the *lattice dimension* of B and denoted $\dim_{\mathrm{L}}(B)$. It is well known, cf. [11], that a graph G has a lattice embedding if and only if G is an isometric subgraph of a hypercube. As the latter is true for benzenoid systems [18], the lattice dimension is well-defined for them.

The paper is organized as follows. In the next section we introduce the concepts needed in this paper, in particular, we define benzenoid systems, present their fundamental trees, and from [2] recall the 3-trees embedding. Then, in Section 3, we give a lower and an upper bound for the lattice dimension of a benzenoid system B. The two bounds are expressed in the number of leaves of the fundamental trees of B and coincide in one half of the cases, while in the other cases they differ by 1. Hence for all practical purposes the proposed labelings are optimal. In Section 4 the labeling algorithm is described. We conclude with an example of the labeling and some remarks.

2 Preliminaries

Benzenoid systems are graphs constructed as follows [12]. Let Z be a circuit on the benzenoid (graphite) lattice. Then a benzenoid system is formed by the vertices and edges of the lattice lying on Z and in the interior of Z. Let e be an edge of a benzenoid system B lying on its perimeter Z. Then the *elementary cut* C_e corresponding to e is the set of all edges of B such that with every edge $f \in C_e$, also the opposite edge with respect to a hexagon containing f belongs to C_e. Note that the set of elementary cuts partitions the edge set of B.

Let B be a benzenoid system. Then its edges can be naturally partitioned into three sets E_1, E_2, and E_3 consisting of (geometrically) parallel edges. In other words, E_i is the union of elementary cuts in the same direction. For $i = 1, 2, 3$ let B_i be the graph obtained from B by removing all the edges of E_i. Let T_i be the graph whose vertices are the connected components of G_i (note that these components are paths), two such components P' and P'' being adjacent in T_i if there are vertices $u \in P'$ and $v \in P''$ such that $uv \in E_i$. Every T_i is a tree, see [2, 4]. We call the trees T_1, T_2, and T_3 the *fundamental trees* of the benzenoid system B. An example of a benzenoid system B, the graphs B_i, and the fundamental trees of B are shown in Figure 1. Chepoi [2] introduced fundamental trees and used them to calculate the diameter of benzenoids system. Later Chepoi and Klavžar [4] followed with a linear time algorithm for computation of the Wiener index.

A graph H is an isometric subgraph of G if $d_H(u, v) = d_G(u, v)$ for any vertices $u, v \in H$. In addition, a graph H *isometrically embeds* into a graph G if H is isomorphic to a subgraph of G.

The *Cartesian product* $G \,\Box\, H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $(a, x)(b, y) \in E(G \,\Box\, H)$ whenever either $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$. The Cartesian product is associative, hence the product of several factors is well-defined. In

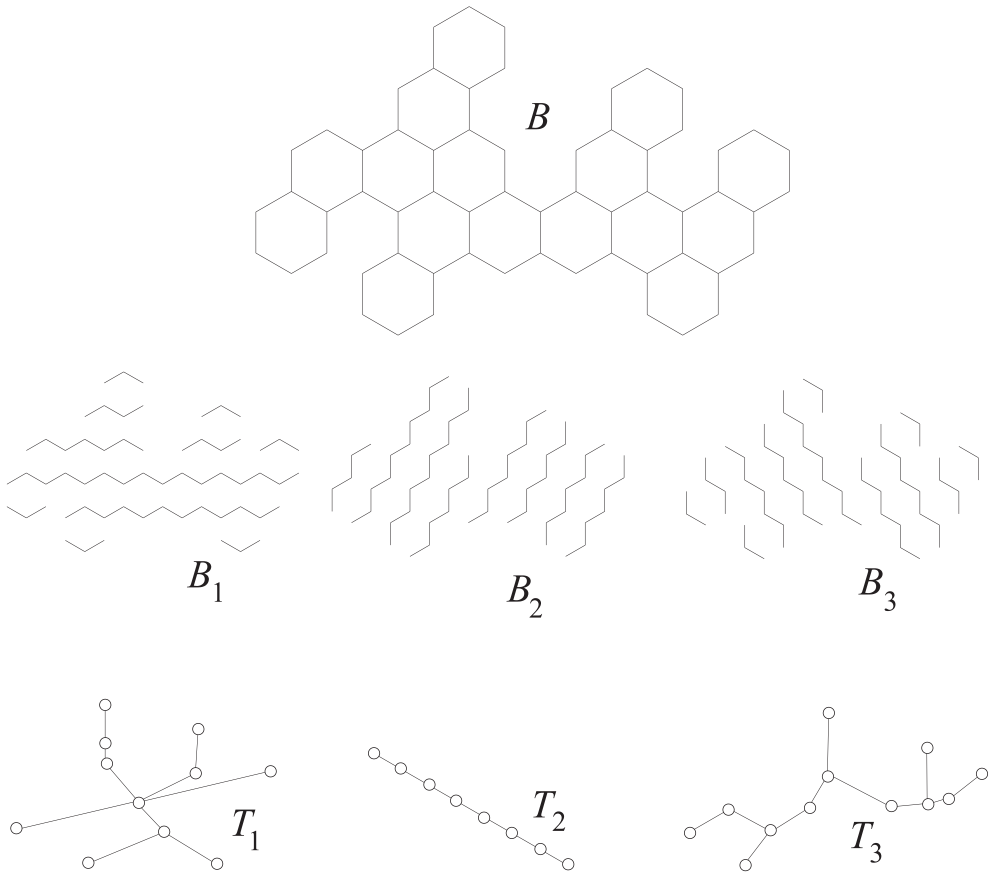

Figure 1: A benzenoid system B, the graphs B_1, B_2, B_3, and the fundamental trees T_1, T_2, T_3

particular, the Cartesian product $T_1 \,\square\, T_2 \,\square\, T_3$ has ordered triples (u_1, u_2, u_3), $u_i \in T_i$, as vertices, and two such triples (u_1, u_2, u_3) and (v_1, v_2, v_3) are adjacent if and only if for some i, $u_i v_i \in E(T_i)$, and $u_j = v_j$ for $j \neq i$.

With these definitions we can now formulate the following result that is essential for our investigations.

Theorem 2.1 (Chepoi [2]) *Let B be a benzenoid system and T_1, T_2, T_3 its fundamental trees. Then B isometrically embeds into the Cartesian product $T_1 \,\square\, T_2 \,\square\, T_3$.*

We recall that the distance function is additive on Cartesian products of graphs, see [17]. More precisely, let G and H be arbitrary graphs, and $(g, h), (g', h')$ vertices of $G \,\square\, H$. Then

$$d_{G \square H}((g, h), (g', h')) = d_G(g, g') + d_H(h, h') \,. \tag{1}$$

Finally, recall that a set of pairwise nonadjacent edges of a graph G is called a *matching* of G.

3 Lattice dimension of benzenoid systems

The infinite benzenoid lattice (also known as the mosaic (6^3)) can be embedded into cubical lattice $\mathbb{Z}^3$, see [8]. Therefore, every benzenoid system which is an isometric subgraph of the infinite benzenoid lattice embeds into $\mathbb{Z}^3$ and has lattice dimension 3. An example of a benzenoid system B that embeds isometrically into $\mathbb{Z}^3$ is shown in Figure 2.

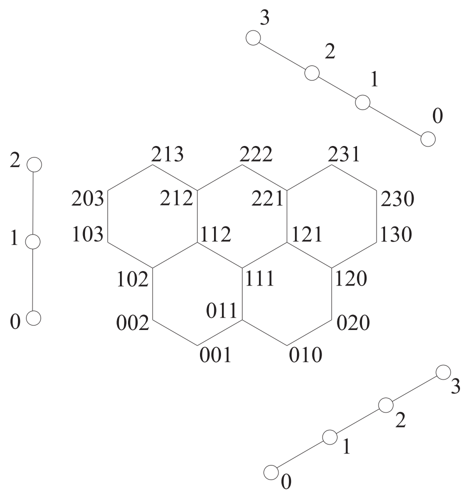

Figure 2: Example of benzenoid system which embeds isometrically into $\mathbb{Z}^3$

However, as soon as B is not isometric in the infinite benzenoid lattice, $\dim_{\mathrm{L}}(B) > 3$. In order to determine the lattice dimension of such benzenoid systems we will use a recent result of Eppstein from [11]. To describe it, the following concepts are needed.

For an edge $e = uv$ of B let W_{uv} and W_{vu} be the connected components of $B \setminus C_e$, where $u \in W_{uv}$ and $v \in W_{vu}$. These subgraphs are called *semicubes* of B. The *semicube graph* $\mathrm{Sc}(B)$ of B is the graph whose vertices are all the semicubes of B, two semicubes W_{uv} and W_{xy} being adjacent if $W_{uv} \cup W_{xy} = B$ and $W_{uv} \cap W_{xy} \neq \emptyset$.

Let B be a benzenoid system. Then its *isometric dimension* $\dim_{\mathrm{I}}(B)$ is the number of elementary cuts of B. In other words, $\dim_{\mathrm{I}}(B) = |\mathrm{Sc}(B)|/2$.

Then Eppstein [11] proved (in a more general setting) the following theorem.

Theorem 3.1 [11] *Let B be a benzenoid system. Then*

$$\dim_{\mathrm{L}}(B) = \dim_{\mathrm{I}}(B) - |M|\,,$$

where M is any maximum matching in $\mathrm{Sc}(B)$.

For our main theorem we need the following three lemmata. A proof of the second one can be found in [1, Lemma 2.3], while the last result has been independently discovered several times, probably for the first time in [16], see also [20].

Lemma 3.2 *Let B be a benzenoid system and W_{uv} a semicube of B. Then W_{uv} is an isolated vertex of* $\mathrm{Sc}(B)$ *if and only if W_{uv} is a leaf of a fundamental tree of B.*

Proof. We observe first that W_{uv} is an isolated vertex of $\mathrm{Sc}(B)$ if and only if no elementary cut of B is completely contained in W_{uv}. Consequently, W_{uv} is an isolated vertex of $\mathrm{Sc}(B)$ if and only if W_{uv} is a path that lies on the perimeter of B. But this is equivalent to the fact that W_{uv} is a leaf of the fundamental tree of B that corresponds to the direction of uv. □

Lemma 3.3 *Let G and H isometric subgraphs of hypercubes. Then* $\dim_{\mathrm{L}}(G \,\square\, H) = \dim_{\mathrm{L}}(G) + \dim_{\mathrm{L}}(H)$.

Since the Cartesian product is associative, Lemma 3.3 holds for any finite number of factors.

Lemma 3.4 *Let T be a tree. Then* $\dim_{\mathrm{L}}(T) = \lceil t/2 \rceil$, *where t is the number of leaves of T.*

Now everything is ready for the next theorem.

Theorem 3.5 *Let B be a benzenoid system and let t_i, $1 \le i \le 3$, be the number of leaves of the fundamental tree T_i. Then*

$$\left\lceil \frac{t_1}{2} + \frac{t_2}{2} + \frac{t_3}{2} \right\rceil \le \dim_{\mathrm{L}}(B) \le \left\lceil \frac{t_1}{2} \right\rceil + \left\lceil \frac{t_2}{2} \right\rceil + \left\lceil \frac{t_3}{2} \right\rceil .$$

Proof. By Theorem 3.1, $\dim_{\mathrm{L}}(B) = \dim_{\mathrm{I}}(B) - |M|$, where M is any maximum matching in $\mathrm{Sc}(B)$. Let r be the number of isolated vertices of $\mathrm{Sc}(B)$. Then

$$|M| \le (|\mathrm{Sc}(B)| - r)/2$$

and by Lemma 3.2 we infer that

$$|M| \le (|\mathrm{Sc}(B)| - (t_1 + t_2 + t_3))/2 .$$

Therefore,

$$\begin{aligned}\dim_{\rm L}(B) &= \dim_{\rm I}(B) - |M| = |{\rm Sc}(B)|/2 - |M| \\ &\geq |{\rm Sc}(B)|/2 - ((|{\rm Sc}(B)| - (t_1 + t_2 + t_3))/2) \\ &= (t_1 + t_2 + t_3)/2\,,\end{aligned}$$

and since the lattice dimension is an integer, the lower bound is proved.

Let B be isometrically embedded into the Cartesian product $T_1 \,\Box\, T_2 \,\Box\, T_3$ of its fundamental trees. Then, B being an isometric subgraph, we infer that $\dim_{\rm L}(B) \leq \dim_{\rm L}(T_1 \,\Box\, T_2 \,\Box\, T_3)$. Therefore, Lemma 3.3 implies that

$$\dim_{\rm L}(B) \leq \dim_{\rm L}(T_1 \,\Box\, T_2 \,\Box\, T_3) = \dim_{\rm L}(T_1) + \dim_{\rm L}(T_2) + \dim_{\rm L}(T_3)\,.$$

Now Lemma 3.4 completes the proof. □

Note that Theorem 3.5 gives the exact lattice dimension of B if at least two of t_1, t_2, and t_3 are even. If at least two of these integers are odd, the theorem approximates the dimension up to 1. So for practical (chemical) purposes the result is completely satisfactory. We do, however, conjecture, that the lower bound is actually always the exact dimension. (See the last example in the final section.) In what follows we use embedding of benzenoid system into Cartesian product of its fundamental trees to obtain lattice coordinates. Thus we always attain the upper bound from Theorem 3.5.

4 Labelling algorithm

Let B be a benzenoid system. As before, let t_i, $1 \leq i \leq 3$, be the number of leaves of the fundamental tree T_i of B. In this section we present a simple procedure how to assigns labels of length

$$r = \left\lceil \frac{t_1}{2} \right\rceil + \left\lceil \frac{t_2}{2} \right\rceil + \left\lceil \frac{t_3}{2} \right\rceil$$

to the vertices of B such that the labeling is a lattice embedding of B into $\mathbb{Z}^r$.

The algorithm first determines the fundamental trees T_1, T_2, and T_3 as described in Section 2. Then, the labeling of B is obtained by simply concatenating the corresponding labelings of the fundamental trees. Hence, it remains to describe an algorithm that labels trees. We review in a simple way the labeling algorithm from [16]. For this some preparation is needed.

Let T be a tree. For vertices u and v of T we denote by $P(u,v)$ the (unique) u,v-path. The *inner degree* of a path of T is defined as $\Sigma_v(\deg(v)-2)$, where the summation runs over the inner vertices of P. Let T' a subtree of T. For a vertex $u \in T \setminus T'$ we define the *u,T'-path* as the path between u and the closest vertex to u that lies in T'.

Let T be a tree with k leaves. We will write $\ell(v) = \ell_1(v)\ell_2(v)\ldots\ell_{\lceil k/2\rceil}(v)$ to denote the label of a vertex v and $\mathbf{e}_i$ for the i-th unit vector (of length $\lceil k/2\rceil$). Now the labeling algorithm can be described as follows.

Algorithm A (Lattice Coordinates of a Tree)

Input: Tree T with k leaves.

Output: Lattice coordinates of vertices of T of length $\lceil k/2\rceil$.

0. Set T' be the empty graph.
1. Find leaves u and v of T such that the inner degree of $P(u,v)$ is maximum.
2. For $x \in P(u,v)$ set $\ell(x) = t0\ldots0$, where $t = d(u,x)$.
3. $T' \leftarrow T' \cup P(u,v)$; $i \leftarrow 2$.
4. While $T' \neq T$ do
   - 4.1. Find leaves u and v of T, $u,v \in T \setminus T'$, such that the inner degrees of the u,T'-path $P(u,y)$ and the v,T'-path $P(v,z)$ are two largest ones.
   - 4.2. For $x \in P(u,y)$ set $\ell(x) = \ell(y) + t\,\mathbf{e}_i$, where $t = d(x,y)$.
   - 4.3. For $x \in P(v,z)$ set $\ell(x) = \ell(z) - t\,\mathbf{e}_i$, where $t = d(x,z)$.
   - 4.4. $T' \leftarrow T' \cup P(u,y) \cup P(v,z)$; $i \leftarrow i+1$.

The coordinatization algorithm needs some comments.

- Note that the vertices y and z from Step 4.1 may coincide.
- If k is odd, then in the last step of the algorithm there is only one leaf left. In this case the path $P(v,z)$ is empty and nothing is done in Step 4.3.
- If we wish to have nonnegative coordinates only, we add to the ith coordinates of labels $-(\min_{v\in T}\ell_i(v))$. We will do so in our example.

To get lattice coordinates of some vertex u of a benzenoid system simply concatenate labels u_1, u_2 and u_3 according to which component of B_i vertex u belongs. That this algorithm indeed produces a lattice embedding follows from Theorem 2.1 and equation (1).

The algorithm from [11] runs in $O(n\tau^2)$ time where n is the number of vertices of a given graphs and τ is equal to the number of elementary cuts. Since fundamental trees can be found in linear time, the complexity of our labeling algorithm is $O(\tau^3)$, that is, the complexity of Algorithm A. So this algorithm is faster than the (general) algorithm from [11]. Moreover, the latter algorithm is rather complicated, since it uses the semicube graphs that are quite clumsy for hand manipulations and one also needs to find maximum matchings in these graphs (which is also nontrivial). On the other hand, our scheme uses only simple concepts.

5 An example and concluding remarks

The benzenoid system from Figure 1 has 28 elementary cuts, hence $\dim_{\mathrm{I}}(B) = 28$. On the other hand, we will now compute that $\dim_{\mathrm{L}}(B) = 7$. Therefore, we need only 7 instead of 28 coordinates.

We first find lattice embeddings of the fundamental trees T_1, T_2 and T_3 of B. We use Algorithm A and show its step-by-step execution on Figure 4. Vertices with already assigned labels at the current stage are colored black. In the last step we add vector 011 to all the labels to get nonnegative coordinates.

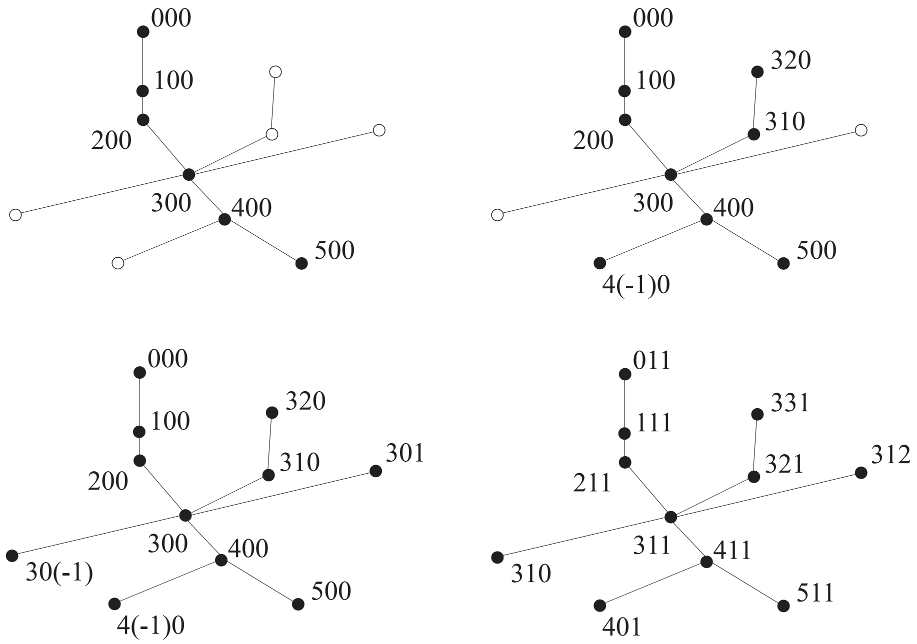

Figure 3: A step-by-step labeling of T_1.

The lattice embeddings of all three fundamental trees are presented in Figure 4, where also the final result is shown—the lattice embedding of B. In the figure the boldface label **4114310** of a vertex from B is obtained by concatenation of the boldface labels **411**, **4**, and **310** from the corresponding fundamental trees.

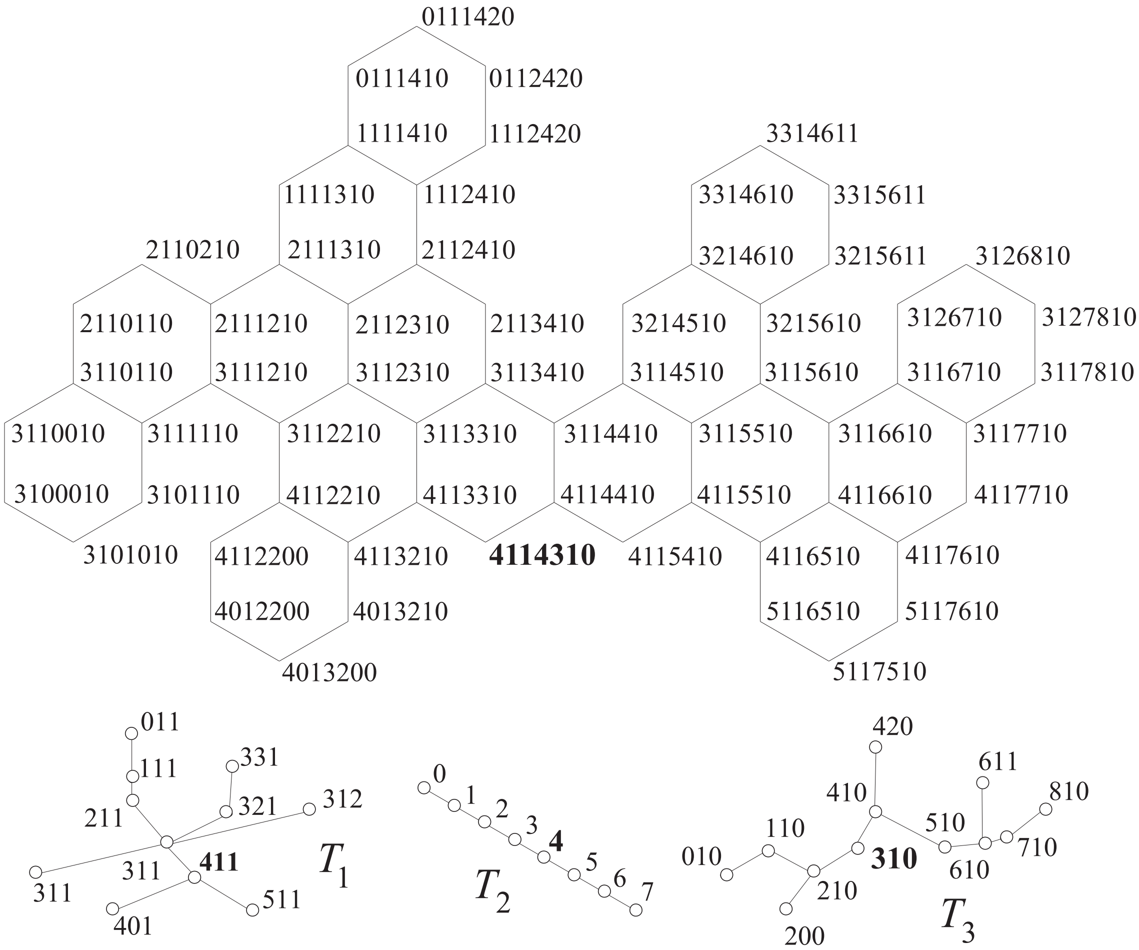

Figure 4: Lattice embedding of B.

We next give the smallest benzenoid system B with the lattice dimension smaller than the dimension found by our algorithm. The system B is shown in Figure 5. Since $\lceil 3/2 \rceil + \lceil 2/2 \rceil + \lceil 3/2 \rceil = 5$, our algorithm finds an embedding into $\mathbb{Z}^5$. On the other hand, $\dim_{\mathrm{L}}(B) = 4$. To see this observe first that for the semicubes W_{uv} and W_{xy} of $\mathrm{Sc}(B)$ (see Figure 5) we have $W_{uv} \cup W_{xy} = B$ and $W_{uv} \cap W_{xy} \neq \emptyset$. Hence they are adjacent in the semicube graph $\mathrm{Sc}(B)$. Moreover, there exists a maximum matching in $\mathrm{Sc}(B)$ including the edge $W_{uv}W_{xy}$ and the remaining edges obtained by embedding trees $T_1 \setminus W_{vu}$ and $T_3 \setminus W_{yx}$ into $\mathbb{Z}$.

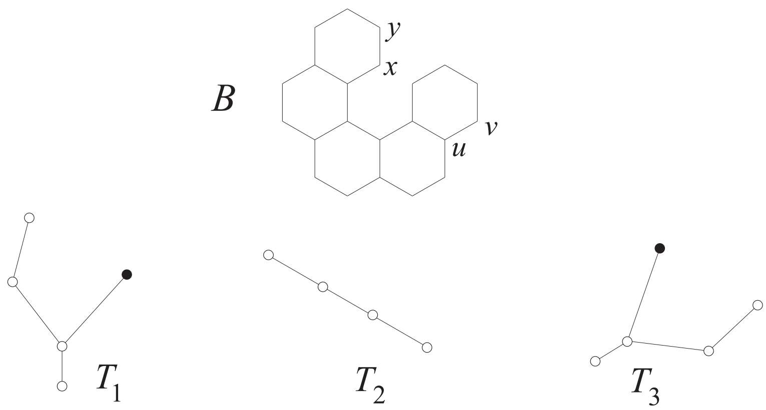

Figure 5: Semicubes W_{vu} and W_{yx} of $\mathrm{Sc}(B)$ correspond to the leaves of the fundamental trees T_1 and T_2 that are colored black.

Similarly we can lower the dimension for one if at least two fundamental trees have an odd number of leaves, where each of the trees has a leaf with the neighbor of degree at least three.

As already mentioned, we conjecture that the lower bound from Theorem 3.5 is actually always the exact dimension. Another natural strengthening of presented results would be to find faster algorithm for lattice embeddings of trees.

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