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Abstract

For a simple graph G with n vertices and m edges, the inequality $M_1(G)/n \leq M_2(G)/m$, where $M_1(G)$ and $M_2(G)$ are the first and the second Zagreb indices of G, is known as Zagreb indices inequality. According to this inequality, a set S of integers is good if for every graph whose degrees of vertices are in S, the inequality holds. We characterize that an interval [a, a + n] is good if and only if $a \geq \frac{n(n-1)}{2}$ or [a, a + n] = [1, 4]. We also present an algorithm that decides if an arbitrary set S of cardinality s is good, which requires $O(s^2 \log s)$ time and O(s) space. Keywords: First Zagreb index, second Zagreb index

1 Introduction

Let G = (V, E) be a simple graph with n = |V| vertices and m = |E| edges. For $v \in V$, d(v) is its degree. The first Zagreb index $M_1(G)$ and the second Zagreb $M_2(G)$ index are defined as follows:

$$M_1(G) = \sum_{v \in V} d(v)^2$$
 and $M_2(G) = \sum_{uv \in E} d(u)d(v).$

For the sake of simplicity, we often use M_1 and M_2 instead of $M_1(G)$ and $M_2(G)$, respectively.

The first and second Zagreb indices are among the oldest topological indices [2, 6, 8], defined in 1972 by Gutman and Trinajstić [7], and are given different names in the literature, such as the Zagreb group indices, the Zagreb group parameters and most often, the Zagreb indices. These indices were among the first indices introduced, and have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. Overall, Zagreb indices exhibit a potential applicability for deriving multi-linear regression models. In 2003 the article [12] repopularized Zagreb indices, and since then a lot of work was done on this topic. For more results on this topic see [4, 5, 11, 16, 17].

Comparing the values of these indices on the same graph is a natural issue and gives interesting results. The following observation suggests that it is more reasonable to compare M_1/n with M_2/m , instead of comparing M_1 with M_2 . Namely, for general graphs, m is bounded from above by n^2 , and thus, the orders of magnitude of M_1 and M_2 are $O(n^3)$ and $O(n^4)$ respectively. At first, the next conjecture was proposed [3]:

Conjecture 1.1. For all simple graphs G,

$$\frac{M_1(G)}{n} \le \frac{M_2(G)}{m} \tag{1}$$

and the bound is tight for complete graphs.

One can easily see that this relation becomes an equality on regular graphs, but also when G is a star. Besides, the inequality is true for trees [14], graphs of maximum degree four, so called chemical graphs [9] and unicyclic graphs [15]. Graphs with only two types of vertex degrees, graphs with vertex degrees in any interval of length three also satisfy the inequality (1), as well as graphs such that their vertices degrees are in the set $\{s - c, s, s + c\}$ or in the interval $[c, c + \lceil \sqrt{c} \rceil]$ for any integers c, s [1]. Here we will determine when a graph with vertices degrees in the interval [a, a + n], satisfies the inequality (1). On the other side there are graphs that do not satisfy the inequality (1), even more, there is an infinite family of graphs of maximum degree $\Delta \geq 5$ such that the inequality. We also present an algorithm for deciding if a given set of integers S of cardinality s satisfy (1), which requires $O(s^2 \log s)$ time and O(s) space.

We denote by $K_{a,b}$ the *complete bipartite* graph with a vertices in one class and b vertices in the other one. Let D(G) be the set of the vertex degrees of G, i.e., $D(G) = \{d(v) \mid v \in V\}$. A set S of integers is good if for every graph G with $D(G) \subseteq S$, the inequality (1) holds. Otherwise, S is a bad set. Since we discuss necessary conditions for (1) to hold, we denote for the sake of simplicity by $m_{i,j}$ the number of edges that connect vertices of degrees i and j in the graph G. Then, as shown in [9]:

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i \le j \\ k \le l \\ (i,j), (k,l) \in \mathbb{N}^2}} \left[\left(i j \left(\frac{1}{k} + \frac{1}{l} \right) + k l \left(\frac{1}{i} + \frac{1}{j} \right) - i - j - k - l \right) m_{i,j} m_{k,l} \right].$$
(2)

Since it makes sense to consider only positive values of the integers i, j, k, l, in the rest of the paper, the term integers will be used for positive integers.

Sometimes in order to examine whether the inequality (1) holds, one can consider whether $M_2/m - M_1/n$ is nonnegative. The difference that we are considering is given by (2). In order to simplify (2), we define a function f, and study some of its properties. Namelly, for integers i, j, k, l, let

$$f(i,j,k,l) = ij\left(\frac{1}{k} + \frac{1}{l}\right) + kl\left(\frac{1}{i} + \frac{1}{j}\right) - i - j - k - l.$$

Now, (2) can be restated as

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i \le j \\ k \le l \\ (i,j), (k,l) \in \mathbb{N}^2}} f(i, j, k, l) m_{i,j} m_{k,l}.$$

Notice that the function f can be represented in the following way

$$f(i, j, k, l) = (ij - kl) \left(\frac{1}{k} + \frac{1}{l} - \frac{1}{i} - \frac{1}{j}\right),$$
(3)

and that it has some symmetry property. For example, for every i, j, k and l:

$$f(i, j, k, l) = f(j, i, k, l)$$
 and $f(i, j, k, l) = f(k, l, i, j).$ (4)

2 Sign of function f

Determining the sign of the function f will help us to see whether the difference $M_2/m - M_1/n$ is nonnegative, and to determine when the inequality (1) holds. By the decomposition (3) of f, the next lemma follows immediately [1].

Lemma 2.1. For any integers i, j, k, l, it holds f(i, j, k, l) < 0 if and only if

(a)
$$ij > kl$$
 and $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$, or
(b) $ij < kl$ and $\frac{1}{k} + \frac{1}{l} > \frac{1}{i} + \frac{1}{j}$.

The next lemma determines the orderings of the integers i, j, k, and l, for which f(i, j, k, l) can be negative [1].

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Lemma 2.2. If f(i, j, k, l) < 0 for some integers $i \leq j$ and $k \leq l$, then,

 $i < k \le l < j$ or $k < i \le j < l$.

The following simple lemma will be used in the proof of Lemma 2.4.

Lemma 2.3. Let $i \leq k \leq l \leq j$ and $k+l \geq i+j$ for some four integers i, j, k, l. Then, $kl \geq ij$.

Proof. Since $k - i \ge j - l$ and j is the largest, we infer $kl - ij = (k - i)j - (j - l)k \ge (j - l)(j - k) \ge 0$. Hence, $kl \ge ij$.

Now, we will present a condition of integers i, j, k, l, for which f(i, j, k, l) is nonnegative.

Lemma 2.4. Let $k + l \ge i + j$ and $i < k \le l < j$ for some four integers i, j, k, l. Then, $f(i, j, k, l) \ge 0$.

Proof. Since $k - i \ge j - l$ by Lemma 2.3, we have $kl \ge ij$, and so

$$\frac{1}{i} + \frac{1}{j} - \frac{1}{k} - \frac{1}{l} = \frac{k-i}{ki} + \frac{l-j}{jl} \ge (j-l)\left(\frac{1}{ki} - \frac{1}{jl}\right) \ge 0.$$

Now the proof is straightforward by Lemma 2.1.

The following proposition gives an equivalence between the sign of f(i, j, k, l) and a relation of the integers i, j, k, l.

Proposition 2.1. Let i, j, k, l be integers satisfying $i < k \le l < j$. Then, f(i, j, k, l) < 0 if and only if $\frac{k+l}{i+j} < \frac{kl}{ij} < 1$.

Proof. First, suppose that $\frac{k+l}{i+j} < \frac{kl}{ij} < 1$. From the left inequality, it follows $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$, and from the right inequality, it follows that ij > kl. Thus, by Lemma 2.1, we have f(i, j, k, l) < 0.

Suppose now that f(i, j, k, l) < 0. By Lemma 2.4, we have that k + l < i + j. If $ij \le kl$, then

$$\frac{1}{k} + \frac{1}{l} - \frac{1}{i} - \frac{1}{j} = \frac{k+l}{kl} - \frac{i+j}{ij} < 0,$$

and by Lemma 2.1, we have $f(i, j, k, l) \ge 0$, which is a contradiction to the assumption. Thus, we may assume that ij > kl, i.e., $\frac{kl}{ij} < 1$. Since f(i, j, k, l) is negative, by Lemma 2.1(a), $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$, and hence $\frac{k+l}{i+j} < \frac{kl}{ij}$. This concludes the proof.

3 Good intervals

It is known that all intervals of lengths 1, 2, 3, and 4, except [2, 5], are good, see [13]. In [1], it was shown that for every integer c, the interval $[c, c + \lceil \sqrt{c} \rceil]$ is good. An immediate corollary of that result is that there are arbitrarily long good intervals. In this section we characterize the good intervals. First we show, if the function is negative for some values of an interval, than that interval is bed.

Proposition 3.1. If f(i, j, k, l) < 0 for some integers $i, j, k, l \in [a, b]$, then [a, b] is a bad interval.

Proof. Whenever f(i, j, k, l) < 0 and $i, j, k, l \in [a, b]$, a > 1, we can construct a connected graph $G_{x,y}$, with $D(G_{x,y}) = \{i, j, k, l\}$, that does not satisfies (1). An illustration of $G_{x,y}$ is given in Figure 1. The construction of $G_{x,y}$ is adapted from [1] and it is as follows:

- Make a sequence of x copies of $K_{i,j}$ and then continue that sequence with y copies of $K_{k,l}$.
- Choose an edge from the first $K_{i,j}$ graph and an edge from the second $K_{i,j}$ graph. Let denote these edges by $v_i^1 v_j^1$ and $v_i^2 v_j^2$, respectively. Replace $v_i^1 v_j^1$ and $v_i^2 v_j^2$ by edges $v_i^1 v_j^2$ and $v_i^2 v_j^1$. Continue this kind of replacement between all consecutive copies of $K_{i,j}$. Notice that these replacements do not change the degrees of the vertices.
- Next, choose an edge from the last $K_{i,j}$ graph and an edge from the first $K_{k,l}$ graph. Let denote these edges by $v_i^x v_j^x$ and $v_k^1 v_l^1$, respectively. Replace $v_i^x v_j^x$ and $v_k^1 v_l^1$ by edges $v_i^x v_l^1$ and $v_k^1 v_j^x$.
- Apply the same procedure between all consecutive graphs $K_{k,l}$ in the sequence. This completes the construction of $G_{x,y}$.



Figure 1: A connected graph $G_{x,y}$ with $D(G_{x,y}) = \{i, j, k, l\}$ constructed from x copies of $K_{k,l}$. The dashed edges are those that are removed from the corresponding complete bipartite graphs.

From the construction, it follows that $m_{i,j} = x \cdot i \cdot j - 1$, $m_{k,l} = y \cdot k \cdot l - 1$, $m_{i,l} = m_{j,k} = 1$

and $m_{i,i} = m_{i,k} = m_{j,j} = m_{j,l} = m_{k,k} = m_{l,l} = 0$. Thus,

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{q \le r, s \le t \\ q, r, s, t \in \{i, j, k, l\}}} f(q, r, s, t) m_{q, r} m_{s, t} \\
= 2 \left[f(i, j, k, l) m_{i, j} m_{k, l} + \left[f(i, j, i, l) + f(i, j, j, k) \right] m_{i, j} \right. \\
\left. + \left[f(k, l, i, l) + f(k, l, j, k) \right] m_{k, l} + f(i, l, j, k) \right].$$

If we increase the number of $K_{i,j}$ and $K_{k,l}$ graphs, i.e., x and y, in the graph $G_{x,y}$, shown in Fig. 1, then $m_{i,j}$ and $m_{k,l}$ will increase as well. Since f(i, j, k, l) < 0, it follows that for $m_{i,j}$ and $m_{k,l}$ big enough, the difference $M_2/m - M_1/n$ will be negative.

Notice that if a = 1 and $\min(i, j, k, l) = 1$, then $G_{x,y}$ is disconnected. Thus, we consider the intervals $[1, b], b \ge 1$, separately. For $1 \le b \le 4$, these intervals are good. The function f(2, 5, 3, 3) is negative, and by the above construction interval [1, b], is bad for every $b \ge 5$. This establish the proposition.

Theorem 3.1. For every integer n, the interval [a, a+n] is good if and only if $a \ge \frac{n(n-1)}{2}$ or [a, a+n] = [1, 4].

Proof. As [1,4] is good interval, in order to prove "if" direction of the theorem, it suffices to show that $f(i, j, k, l) \ge 0$ whenever $i, j, k, l \in [a, a + n]$ and $a \ge \frac{n(n-1)}{2}$. Suppose in contrary that, by Proposition 3.1 for some i, j, k, l from such an interval, f(i, j, k, l) < 0. By Lemma 2.2 and (4), we can assume that $a \le i < k \le l < j \le a + n$. Let k = i + s, l = i + t, j = i + q, where $0 < s \le t < q \le n$. Now,

$$\frac{1}{k} + \frac{1}{l} = \frac{2i+s+t}{(i+s)(i+t)} \qquad \text{and} \qquad \frac{1}{i} + \frac{1}{j} = \frac{2i+q}{i(i+q)}.$$

Since f(i, j, k, l) < 0, by Proposition 2.1, it follows that kl < ij and k + l < i + j. Thus, we obtain s + t < q. As, $st \le \frac{(s+t)^2}{4}$, we obtain $st \le \frac{(q-1)^2}{4} \le \frac{(n-1)^2}{4}$. By Lemma 2.1, it follows that f(i, j, k, l) < 0 if $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$. Hence,

$$\begin{array}{rcl} \displaystyle \frac{2i+s+t}{(i+s)(i+t)} &< \displaystyle \frac{2i+q}{i(i+q)} \\ (2i+s+t)(i^2+iq) &< \displaystyle (2i+q)(i^2+(s+t)i+st) \\ \\ \displaystyle 2i^3+(s+t+2q)i^2+(s+t)iq &< \displaystyle 2i^3+(2s+2t+q)i^2+2sti+(s+t)iq+stq \\ \\ \displaystyle q\,i^2 &< \displaystyle (s+t)\,i^2+2s\,t\,i+s\,t\,q \\ \\ \displaystyle q\,i^2 &< \displaystyle (q-1)\,i^2+2s\,t\,i+s\,t\,q, \end{array}$$

from here

$$\begin{aligned} i^2 &< 2st\,i + st\,q\\ &\leq 2\left(\frac{n-1}{2}\right)^2 i + \left(\frac{n-1}{2}\right)^2 n\\ &\leq 2\left(\frac{n-1}{2}\right)^2 i + \frac{n-1}{2}i\\ &\leq i\frac{n(n-1)}{2}, \end{aligned}$$

which is clearly impossible. Thus, we have shown that $f(i, j, k, l) \ge 0$ for arbitrary i, j, k, lfrom an interval [a, a + n] with $a \ge \frac{n(n-1)}{2}$. Therefore, such an interval is a good one.

Now, we prove the opposite direction. For n = 0, 1, 2 and an arbitrary integer a, all intervals [a, a+n] are good, see [13], and they satisfy the inequality $a \ge \frac{n(n-1)}{2}$. For n = 3, [1, 4] is the only good interval that does not satisfy $a \ge \frac{n(n-1)}{2}$.

For $n \ge 4$, we proceed as follows. By Proposition 3.1, it suffices to show that f(i, j, k, l) < 0 for some integers $i, j, k, l \in [a, a + n]$, and $a \in A_n = \left\{1, 2, 3, \dots, \binom{n}{2} - 1\right\}$. We show this by induction on n.

For the base of the induction, n = 4, we have a < 6, and the intervals of interest are [1,5], [2,6], [3,7], [4,8], and [5,9]. Functions f(2,5,3,3), f(3,7,4,5), f(4,8,5,6), and f(5,9,6,7) are negative, and each corresponds to at least one of the above intervals.

By induction hypothesis, we can assume that, for $n-1 \ge 4$ and $a \in A_{n-1}$, the interval [a, a+n-1] is bad.

Now, we show that for n and $a \in A_n$ the interval [a, a + n] is bad. First, notice that $A_{n-1} \subset A_n$. Suppose first $a \in A_{n-1}$. Since [a, a + n - 1] is a subinterval of [a, a + n], and by induction hypothesis [a, a + n - 1] is a bad interval, it follows that also [a, a + n] is bad.

It remains to show that [a, a + n] is a bad interval for $a \in A_n \setminus A_{n-1}$, i.e., for $a \in \left[\frac{(n-1)(n-2)}{2}, \frac{n(n-1)}{2}\right]$. We consider two cases regarding the parity of n:

• n = 2s + 1: Then, $2s^2 - s \le a < 2s^2 + s$. Now, it can be easily verified that

$$f(a, a + 2s + 1, a + s, a + s) = \frac{(a - s - 2s^2)(a - s^2)}{a(a + s)(a + 2s + 1)} < 0.$$

• n = 2s: Then, $(s-1)(2s-1) \le a < s(2s-1)$. Again, an easy verification shows that

$$f(a, a+2s, a+s-1, a+s) = \frac{(a-s^2+s)(a^2+2as+2s^2-2as^2-2s^3)}{a(a+2s)(a+s-1)(a+s)} < 0.$$

Thus, the proof is completed.

4 Decision algorithm

In this section, we consider a problem of deciding if a given set of integers S of cardinality s is a good one.

A straightforward algorithm that solves the above problem is to check if f(i, j, k, l) < 0for all 4-tuples (i, j, k, l) from S, where the 4-tuples (i, j, k, l) are variations with repetitions. Checking that suffices to determine if S is good or not, since by Proposition 3.1, if f(i, j, k, l) < 0, we can construct a graph that does not satisfy (1). Verifying if f(i, j, k, l) < 0 can be done in constant time by Lemma 2.1. Thus, the time complexity of this approach is $O(s^4)$.

We now show that, using quite simple algorithmic tricks, one can obtain an $O(s^2 \log s)$ algorithm.

Lemma 4.1. There exists an algorithm that checks whether a given set of positive integers S is good and requires $O(s^2 \log s)$ time and $O(s^2)$ space.

Proof. Let us denote $P_1(i, j) = ij$ and $P_2(i, j) = \frac{1}{i} + \frac{1}{j}$. From (3) we obtain that f(i, j, k, l) < 0 if and only if $P_1(i, j) < P_1(k, l)$ and $P_2(i, j) < P_2(k, l)$ or $P_1(i, j) > P_1(k, l)$ and $P_2(i, j) > P_2(k, l)$. Using the symmetry of the function f, the set S is good if and only if for each pair $(k, l) \in S \times S$ there does not exist a pair $(i, j) \in S \times S$ such that both $P_1(i, j) < P_1(k, l)$ and $P_2(i, j) < P_2(k, l)$.

Let us assing $P(i,j) = (P_1(i,j) - P_2(i,j))$ and compare values P(i,j) lexicographically (that is, P(i,j) < P(k,l) if $P_1(i,j) < P_1(k,l)$ or $P_1(i,j) = P_1(k,l)$ and $-P_2(i,j) < -P_2(k,l)$, i.e., $P_2(i,j) > P_2(k,l)$). Note that now the set S is good if and only if for each two pairs $(i,j), (k,l) \in S \times S$ if P(i,j) < P(k,l) then $P_2(i,j) \ge P_2(k,l)$.

The algorithm, sketched in Pseudocode 4.1, simply checks the above condition. We sort all pairs $(i, j) \in S \times S$ increasingly according to the value of P(k, l) and then iterate over the sorted array T and check if there exist consecutive values (k', l') and (k, l) such that $P_2(k', l') < P_2(k, l)$. If we found such values, we have $P_1(k', l') < P_1(k, l)$ since $P(k', l') \le$ P(k, l), and the set S is not good. Otherwise, we find that the array is sorted nonincreasingly according to P_2 and, thus, if for any $(i, j), (k, l) \in S \times S$ we have $P_1(i, j) < P_1(k, l)$ then P(i, j) < P(k, l) and $P_2(i, j) \ge P_2(k, l)$, and, finally, the set S is good.

Note that in Pseudocode 4.1 we do not keep the indices (k', l') of the previously considered pair, but we only store the value $P_2(k', l')$ in the variable p_2 .

Let us now analyze consumed time and space. The sorting according to the value of P consumes $O(s^2 \log s)$ time if we use Merge Sort or Heap Sort. We use $O(s^2)$ space to store the sorted pairs in the array T.

The space complexity can be further improved to O(s). Note that in the algorithm from Lemma 4.1 we do not need to actually store the table T — we need only to iterate over pairs (k, l) in the increasing order of $P(k, l) = (P_1(k, l), -P_2(k, l))$. The following technical lemma shows that such iterator can be constructed using O(s) space and $O(s^2 \log s)$ total time.

Lemma 4.2. There exists an algorithm that, given a set S of s positive integers, generates a sequence of pairs $(k,l) \in S \times S$ in the increasing order of $P(k,l) = (P_1(k,l), -P_2(k,l))$. It uses O(s) additional space and $O(s^2 \log s)$ total time.

Algorithm 4.1 An $O(s^2 \log s)$ algorithm that checks whether S is a good set.	
1:	procedure $CHECKGOODSET(S)$
2:	$T \leftarrow \text{the set of all pairs } (k,l) \in S \times S$
3:	sort T in the increasing order of $P(k, l) = (P_1(k, l), -P_2(k, l))$
4:	$p_2 \leftarrow \infty$
5:	for each pair $(k, l) \in T$ in the increasing order of $P(k, l)$ do
6:	$\mathbf{if} \ p_2 < P_2(k,l) \ \mathbf{then}$
7:	return NO
8:	$p_2 \leftarrow P_2(k,l)$
9:	return YES

Proof. First observe that for each $k \in S$, if l < l', the algorithm should first provide the pair (k, l) before the pair (k, l'). Thus, for a fixed k, the pairs (k, l) should be generated in the increasing order of l.

We make use of this observation in the algorithm described in Pseudocode 4.2. In the initialization part we first sort the set S and store it in an array $S[1 \dots s]$. The algorithm uses a standard binary heap that stores pairs of indices $(a, b) \in \{1, 2, \dots, s\} \times \{1, 2, \dots, s\}$ and sorts them according to the key P(S[a], S[b]). A pair (a, b) in the heap means that the algorithm has not yet generated pair (S[a], S[b]), but has already generated all pairs (S[a], S[b']) for $1 \leq b' < b$. Thus, for each a, the heap contains the pair (a, b) that corresponds to the pair (S[a], S[b]) that should be the first generated pair with S[a] on the first coordinate. At each step of the iterator (i.e., at each call to the NEXTPAIR procedure) we simply return the minimum element of the heap H and update the heap.

The initialization costs $O(s \log s)$ time and uses O(s) space for the array $S[1 \dots s]$. At every time there is at most one pair (a, b) for each $1 \leq a \leq s$ stored in the heap H, so the heap H uses O(s) space. Each call to NEXTPAIR results in a few operations on the heap H, thus each call needs $O(\log s)$ time. In total, we consumed $O(s^2 \log s)$ time to generate all pairs.

Algorithm 4.2 An iterator of pairs $(k, l) \in S$ in the increasing order of $P(k, l)$.		
1:	procedure INITIALIZEITERATOR (S)	
2:	$S[1\dots s] \leftarrow \text{sorted set } S$	
3:	$H \leftarrow$ an empty binary heap, storing pairs of integers (a, b) , and sorting according to	
	key $P(S[a], S[b])$, with the smallest key on the top	
4:	for $a := 1$ to s do	
5:	$H \leftarrow H \cup (a, 1)$	
6:	procedure NextPair	
7:	$(a,b) \leftarrow \text{minimum element of } H$	
8:	remove the minimum element of H	
9:		
10:	$H \leftarrow H \cup (a, b+1)$	
11:	$\mathbf{return} \ (S[a], S[b])$	

Combining Lemma 4.1 and Lemma 4.2 we obtain the final theorem.

Theorem 4.1. There exists an algorithm that checks whether a given set of positive integers S is good and requires $O(s^2 \log s)$ time and O(s) space.

Proof. We use the algorithm of Lemma 4.1, but instead of the array T we use iterator described in Lemma 4.2. Thus, in Line 5 of Pseudocode 4.1 we repeatedly call the procedure NEXTPAIR instead of iterating over the array T.

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