Graphs that are Not Pairwise Compatible: A New Proof Technique (Extended Abstract)*

Pierluigi Baiocchi, Tiziana Calamoneri, Angelo Monti, and Rossella Petreschi

Computer Science Department,
"Sapienza" University of Rome, Italy
calamo/monti/petreschi@di.uniroma1.it,
pierluigi.baiocchi@gmail.com

Abstract. A graph $G = (V, E)$ is a *pairwise compatibility graph* (PCG) if there exists an edge-weighted tree T and two non-negative real numbers d_{min} and d_{max}, $d_{min} \leq d_{max}$, such that each node $u \in V$ is uniquely associated to a leaf of T and there is an edge $(u, v) \in E$ if and only if $d_{min} \leq d_T(u, v) \leq d_{max}$, where $d_T(u, v)$ is the sum of the weights of the edges on the unique path $P_T(u, v)$ from u to v in T. Understanding which graph classes lie inside and which ones outside the PCG class is an important issue. Despite numerous efforts, a complete characterization of the PCG class is not known yet. In this paper we propose a new proof technique that allows us to show that some interesting classes of graphs have empty intersection with PCG. We demonstrate our technique by showing many graph classes that do not lie in PCG. As a side effect, we show a not pairwise compatibility planar graph with 8 nodes (i.e. C_8^2), so improving the previously known result concerning the smallest planar graph known not to be PCG.

Keywords: Phylogenetic Tree Reconstruction Problem, Pairwise Compatibility Graphs (PCGs), PCG Recognition Problem.

1 Introduction

Graphs we deal with in this paper are motivated by a fundamental problem in computational biology, that is the reconstruction of ancestral relationships. It is known that the evolutionary history of a set of organisms is represented by a *phylogenetic tree*, i.e. a tree where leaves represent distinct known taxa while internal nodes are possible ancestors that might have led through evolution to this set of taxa. The edges of the tree are weighted in order to represent a kind of evolutionary distance among species. Given a set of taxa, the *phylogenetic tree reconstruction problem* consists in finding the "best" phylogenetic tree that explains the given data. Since it is not completely clear what "best" means, the

* Partially supported by *Sapienza* University of Rome projects "Graph Algorithms for Phylogeny: a promising approach" and "Combinatorial structures and algorithms for problems in co-phylogeny".

performance of the reconstruction algorithms is usually evaluated experimentally by comparing the tree produced by the algorithm with those partial subtrees that are unanimously recognized as "sure" by biologists. However, the tree reconstruction problem is proved to be NP-hard under many criteria of optimality, moreover real phylogenetic trees are usually huge, so testing these heuristics on real data is in general very difficult. This is the reason why it is common to exploit *sample techniques*, extracting relatively small subsets of taxa from large phylogenetic trees, according to some biologically-motivated constraints, and to test the reconstruction algorithms only on the smaller subtrees induced by the sample. The underlying idea is that the behavior of the algorithm on the whole tree will be more or less the same as on the sample. It has been observed that using, in the sample, very close or very distant taxa can create problems for phylogeny reconstruction algorithms [9] so, in selecting a sample from the leaves of the tree, the constraint of keeping the distance between any two leaves in the sample between two given positive integers d_{min} and d_{max} is used. This motivates the introduction of *pairwise compatibility graphs* (PCG). Indeed, given a phylogenetic tree T and integers d_{min}, d_{max}, we can associate a graph G, called the pairwise compatibility graph of T, whose nodes are the leaves of T and for which there is an edge between two nodes if the corresponding leaves in T are at a weighted distance within the interval $[d_{min}, d_{max}]$.

From a more theoretical point of view, we highlight that the problem of sampling a set of m leaves from a weighted tree T, such that their distance is within some interval $[d_{min}, d_{max}]$, reduces to selecting a clique of size m uniformly at random from the associated pairwise compatibility graph. As the sampling problem can be solved in polynomial time on PCGs [10], it follows that the *max clique problem* is solved in polynomial time on this class of graphs, if the edge-weighted tree T and the two values d_{min}, d_{max} are known or can be provided in polynomial time.

The previous reasonings motivate the interest of researchers in the so called *PCG recognition problem*, consisting in understanding whether, given a graph G, it is possible to determine an edge-weighted tree T and two integers d_{min}, d_{max} such that G is the associated pairwise compatibility graph; in this case G can be briefly denoted as $PCG(T, d_{min}, d_{max})$.

Figure 1.a depicts a graph that is $PCG(T, 4, 5)$, where T is shown in Figure 1.b. In general, T is not unique; here T is a *caterpillar*, i.e. a tree consisting of a central path, called spine, and nodes directly connected to that path. Due to their simple structure, caterpillars are the most used witness trees to show that a graph is PCG. However, it has been proven that there are some PCGs for which it is not possible to find a caterpillar as witness tree [5].

Due to the flexibility afforded in the construction of instances (i.e. choice of tree topology and values for d_{min} and d_{max}), when PCGs were introduced, it was also conjectured that all graphs are PCGs [10]. This conjecture has been refuted by proving the existence of some graphs not belonging to PCG. Namely, Yanhaona et al. [13] show a bipartite not PCG with 15 nodes. Mehnaz and Rahman [11] generalize the technique in [13] to provide a class of bipartite graphs

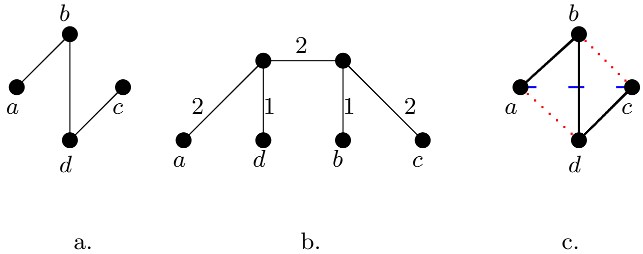


Fig. 1. a. A graph G. b. An edge-weighted caterpillar T such that $G = PCG(T, 4, 5)$. c. G where the PCG-coloring induced by triple $T, 4, 5$ is highlighted.

that are not PCGs. More recently, Durocher et al. [8] prove that there exists a not bipartite graph with 8 nodes that is not PCG; this is the smallest not planar graph that is not pairwise compatibility, since all graphs with at most 7 nodes are PCGs [5]. The authors of [8] provide also an example of a planar graph with 20 nodes that is not PCG. Moreover, it holds that, if a graph H is not a PCG, then every graph admitting H as an induced subgraph is also not a PCG [6]. Finally, a graph is not PCG if its complement has two 'far' induced subgraphs which are either a chordless cycle of at least four nodes or the complement of a cycle of length at least 5; two induced subgraphs are 'far' if they are both node disjoint and there is no edge connecting them [15] .

From the other side, many graph classes have been proved to be in PCG, such as cliques and trees, cycles, single chord cycles, cacti, tree power graphs [14, 13], interval graphs [3], triangle-free outerplanar 3-graphs [12] and Dilworth 2 graphs [7].

However, despite these results, the exact boundary of the PCG class remains unclear. In this paper, we move a concrete step in the direction of searching new graph classes that are not PCGs. To this aim, in Section 2 we introduce a new proof technique that allows us to show that some interesting classes have empty intersection with PCG. In particular, in Section 3 we show in detail the application of this technique on the class of graphs constructed as the square of a cycle. We prove that, for every $n \geq 8$, C_n^2 is not a PCG. Moreover, we show that by deleting any node from C_n^2 we get a PCG, thus proving that it does not contain any induced subgraph that is not PCG, i.e. we prove that C_n^2 is a *minimal* graph that is not PCG.

As a side effect, we prove that there exists also an 8 node planar graph that is not PCG, i.e. C_8^2, so improving the known result of a not pairwise compatibility planar graph with 20 nodes.

Finally, in Section 4, we present two other classes of graphs, obtained by modifying cycle graph in different ways, and we show that they are not PCGs through the application of our technique.

Due to the lack of space, for these latter classes, we only state the results referring the reader to [1] for the proofs' details.

2 Proof Technique

In this section, after introducing some definitions, we describe our proof technique, useful to prove that some classes of graphs have empty intersection with the class of PCGs, formally defined as follows.

Definition 1. *[10] A graph $G = (V, E)$ is a* pairwise compatibility graph *(PCG) if there exists a tree T, a weight function assigning a positive real value to each edge of T, and two non-negative real numbers d_{min} and d_{max} with $d_{min} \leq d_{max}$, such that each node $u \in V$ is uniquely associated to a leaf of T and there is an edge $(u, v) \in E$ if and only if $d_{min} \leq d_T(u, v) \leq d_{max}$, where $d_T(u, v)$ is the sum of the weights of the edges on the unique path $P_T(u, v)$ from u to v in T.*

All trees in this paper are edge-weighted.

Given a graph $G = (V, E)$, we call *non-edges* of G the edges that do not belong to the graph. A *tri-coloring of* G is an edge labeling of the complete graph $K_{|V|}$ with labels from set { black, red, blue } such that all edges of $K_{|V|}$ that are in G are labeled black, while all the other edges of $K_{|V|}$ (i.e. the non-edges of G) are labeled either red or blue. A tri-coloring is called a *partial tri-coloring* if not all the non-edges of G are labeled.

Notice that, if $G = PCG(T, d_{min}, d_{max})$, some of its non-edges do not belong to G because the weights of the corresponding paths on T are strictly larger than d_{max}, while some other edges are not in G because the weights of the corresponding paths on T are strictly smaller than d_{min}. This motivates the following definition.

Definition 2. *Given a graph $G = PCG(T, d_{min}, d_{max})$, we call its* PCG-coloring *the tri-coloring $\mathcal{C}$ of G such that:*
- (u, v) is red *in $\mathcal{C}$ if $d_T(u, v) < d_{min}$,*
- (u, v) is black *in $\mathcal{C}$ if $d_{min} \leq d_T(u, v) \leq d_{max}$,*
- (u, v) is blue *in $\mathcal{C}$ if $d_T(u, v) > d_{max}$.*
In such a case, we will say that triple (T, d_{min}, d_{max}) induces *the PCG-coloring $\mathcal{C}$.*

In order to read the figures even in gray scale, we draw red edges as red-dotted and blue edges as blue-dashed in all the figures.

In Figure 1.c we highlight the PCG-coloring induced by the triple $(T, 4, 5)$ where T is the tree in Figure 1.b.

The following definition formalizes that not all tri-colorings are PCG-colorings.

Definition 3. *A tri-coloring $\mathcal{C}$ (either partial or not) of a graph G is called a* forbidden PCG-coloring *if no triple (T, d_{min}, d_{max}) inducing $\mathcal{C}$ exists.*

Observe that a graph is PCG if and only if there exists a tri-coloring $\mathcal{C}$ that is a PCG-coloring for G. Besides, any induced subgraph H of a given $G = PCG(T, d_{min}, d_{max})$ is also PCG, indeed $H = PCG(T', d_{min}, d_{max})$, where T' is the subtree induced by the leaves corresponding to the nodes of H. Moreover,

H inherits the PCG-coloring induced by triple (T, d_{min}, d_{max}) from G. Thus, if we were able to prove that H, although PCG, inherits a forbidden PCG-coloring from a tri-coloring $\mathcal{C}$ of G, then we would show that $\mathcal{C}$ cannot be a PCG-coloring for G in any way. This is the core of our proof technique:

Given a graph G that we want to prove not to be PCG:

1. *list some forbidden PCG-colorings of particular graphs that are induced subgraphs of G;*
2. *show that each tri-coloring of G induces a forbidden PCG-coloring in at least an induced subgraph;*
3. *conclude that G is not PCG, since all its tri-colorings are proved to be forbidden.*

3 The square of a cycle

In this section we exploit the proof technique just described on a particular class of graphs, i.e. the square of a cycle; we recall that the square G^2 of a graph G is a new graph whose node set coincides with the node set of G, and an edge (u, v) is in G^2 if either (u, v) is in G or (u, w) and (w, v) are both in G for some node w.

3.1 Forbidden tri-colorings of some subgraphs of C_n^2

In agreement with the proof technique described in Section 2, as a first step, here we highlight forbidden partial tri-colorings of paths P_n, $n \geq 3$ and cycles C_n, $n \geq 4$. Moreover, we prove forbidden colorings and partial forbidden colorings (for short **f-c**) for some graphs that are induced subgraphs of C_n^2 (see Figures 2 and 3).

Given a graph $G = (V, E)$ and a subset $S \subseteq V$, we denote by $G[S]$ the subgraph of G induced by nodes in S.

A *subtree induced by a set of leaves* of T is the minimal subtree of T which contains those leaves. In particular, we denote by T_{uvw} the subtree of a tree induced by three leaves u, v and w.

The following lemma from [13] will be largely used:

Lemma 1. *Let T be a tree, and u, v and w be three leaves of T such that $d_T(u, v) \geq \max\{d_T(u, w), d_T(v, w)\}$. Let x be a leaf of T other than u, v, w. Then, $d_T(w, x) \leq \max\{d_T(u, x), d_T(v, x)\}$.*

It is known that P_m is a PCG [14]; the following lemma gives some constraints to the associated PCG-coloring.

Lemma 2. *Let P_m, $m \geq 4$, be path $v_1, \ldots, v_m$ and let $\mathcal{C}$ be one of its PCG-colorings. If all non-edges (v_1, v_i), $3 \leq i \leq m-1$, and (v_2, v_m) are colored with blue in $\mathcal{C}$, then also non-edge (v_1, v_m) is colored with blue in $\mathcal{C}$.*

Proof. Let $\mathcal{C}$ be the PCG-coloring of P_m induced by triple (T, d_{min}, d_{max}). We apply Lemma 1 iteratively.

First consider nodes v_1, v_2, v_3 and v_4 as u, w, v and x: $P_T(v_1, v_3)$ is easily the largest path in $T_{v_1 v_3 v_2}$; then $d_T(v_2, v_4) \leq \max\{d_T(v_1, v_4), d_T(v_3, v_4)\} = d_T(v_1, v_4)$. This is because (v_1, v_4) is a blue non-edge by hypothesis while (v_3, v_4) is an edge.

Now repeat the reasoning with nodes v_1, v_2, v_i and v_{i+1}, $4 \leq i < m$, as u, w, v and x, exploiting that at the previous step we have obtained that $d_T(v_2, v_i) \leq d_T(v_1, v_i)$: in $T_{v_1 v_i v_2}$, $P_T(v_1, v_i)$ is the largest path and so
$d_T(v_2, v_{i+1}) \leq \max\{d_T(v_1, v_{i+1}), d_T(v_i, v_{i+1}) = d_T(v_1, v_{i+1})$ since (v_1, v_{i+1}) is a blue non-edge while (v_i, v_{i+1}) is an edge.

Posing $i = m - 1$, we get that $d_T(v_2, v_m) \leq d_T(v_1, v_m)$; since non-edge (v_2, v_m) is blue by hypothesis, (v_1, v_m) is blue, too. □

Given a graph, in order to ease the exposition, we call *2-non-edge* a non-edge between nodes that are at distance 2 in the graph.

Lemma 3. *Let P_n, $n \geq 3$, be a path. Any PCG-coloring of P_n that has at least one red non-edge but no red 2-non-edges is forbidden.*

Proof. If $n = 3$, there is a unique non-edge and it is a 2-non-edge; so, the claim trivially follows.

So, let it be $n \geq 4$ and consider a triple (T, d_{min}, d_{max}) inducing a PCG-coloring with at least a red non-edge. Among all red non-edges, let (v_i, v_j) – $i < j$– be the one such that $j - i$ is minimum. Assume by contradiction, $j - i > 2$. Consider now the subpath P' induced by $v_i, \ldots, v_j$. P' has at least 4 nodes and inherits the PCG-coloring from P_n; in it, there is only a red non-edge (i.e. the non-edge connecting v_i and v_j). P' satisfies the hypothesis of Lemma 2, hence (v_i, v_j) must be blue, against the hypothesis that it is red. □

Lemma 4. *Let C_n, $n \geq 4$, be a cycle. Then any PCG-coloring of C_n that does not have red 2-non-edges is forbidden.*

Proof. Let $C_n = PCG(T, d_{min}, d_{max})$, $n \geq 4$; from [14], at least a non-edge (u, v) such that $d_T(u, v) < d_{min}$. In our setting, this means that every PCG-coloring of C_n, $n \geq 4$, has at least one red non-edge. By contradiction, w.l.o.g. assume that this non-edge is (v_1, v_i), with $4 \leq i < n - 1$. We apply Lemma 3 on the induced P_i and the claim follows. □

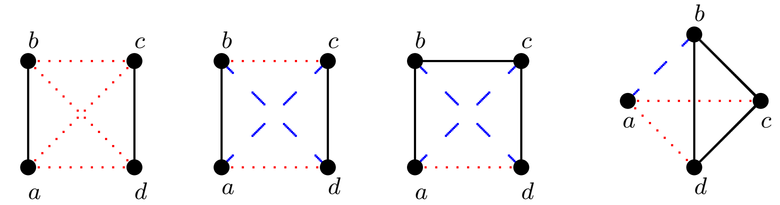
Lemma 5. *The tri-colorings in Figure 2 are forbidden PCG-colorings.*

Proof. We prove separately that each tri-coloring is forbidden.

Forbidden tri-coloring f-c$(2K_2)a$:

We obtain that the tri-coloring in Figure 2.a is forbidden by rephrasing Lemma 6 of [8] with our nomenclature.

The other proofs are all by contradiction and proceed as follows: for each tri-coloring in Figure 2, we assume that it is a feasible PCG-coloring induced by a triple (T, d_{min}, d_{max}) and show that this assumption contradicts Lemma 1.



a. **f-c**$(2K_2)a$ b. **f-c**$(2K_2)b$ c. **f-c**(P_4) d. **f-c**$(K_3 \cup K_1)$

Fig. 2. Forbidden tri-colorings of some graphs.

Forbidden tri-coloring f-c$(2K_2)b$:

From the tri-coloring in Figure 2.b we have that

$$d_T(b,c) < d_{min} \le d_T(a,b) \le d_{max} < d_T(a,c).$$

Thus $P_T(a,c)$ is the largest path in $T_{a,b,c}$. By Lemma 1, for leaf d it must be: $d_T(b,d) \le \max\{d_T(a,d), d_T(c,d)\} = d_T(c,d)$ while from the tri-coloring it holds that $d_T(c,d) \le d_{max} < d_T(b,d)$, a contradiction.

Forbidden tri-coloring f-c(P_4):

From the tri-coloring in Figure 2.c we have that

$$d_T(a,b), d_T(b,c) \le d_{max} < d_T(a,c).$$

Thus $P_T(a,c)$ is the largest path in $T_{a,b,c}$. By Lemma 1, for leaf d we have: $d_T(b,d) \le \max\{d_T(a,d), d_T(c,d)\} = d_T(c,d)$ while from the tri-coloring it holds that $d_T(c,d) \le d_{max} < d_T(b,d)$, a contradiction.

Forbidden tri-coloring f-c$(K_3 \cup K_1)$:

From the tri-coloring in Figure 2.d we have that

$$d_T(a,d), d_T(a,c) < d_{min} \le d_T(c,d).$$

Thus $P_T(c,d)$ is the largest path in $T_{a,c,d}$. By Lemma 1, for leaf b it must be: $d_T(a,b) \le \max\{d_T(c,b), d_T(d,b)\}$ while from the tri-coloring it holds that $d_T(c,b), d_T(d,b) < d_{max} \le d_T(a,b)$, a contradiction. □

Lemma 6. *The partial tri-coloring in Figure 3 is a forbidden PCG-coloring.*

Proof. Using the result of Lemma 5, we again prove that each tri-coloring is forbidden by contradiction.

From the the tri-coloring in Figure 3, extract the inherited PCG-colorings for the two subgraphs $G[a,c,d,e]$ and $G[b,c,d,f]$. To avoid **f-c**$(K_3 \cup K_1)$, the non-edges (a,e) and (b,f) are both blue. Now we distinguish the two possible cases for the color of the non-edge (a,f):

(a,f) **is a red non-edge:** consider the PCG-coloring for subgraph $G[a,b,e,f]$. To avoid **f-c**$(2K_2)b$, non-edge (b,e) has to be blue. This implies that the PCG-coloring for path $G[a,b,d,e,f]$ has all the 2-non-edges with color blue while the non-edge (a,f) is red. This is in contradiction with Lemma 3.

(a,f) **is a blue non-edge:** in this case consider Lemma 1 applied to tree $T_{a,d,f}$. We distinguish the three cases for the largest path among $P_T(a,d)$, $P_T(a,f)$ and $P_T(d,f)$:

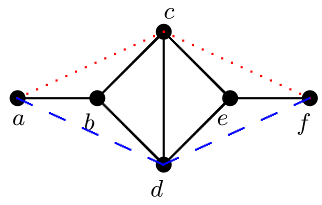


Fig. 3. A forbidden coloring of a graph that is an induced subgraph of C_n^2, with $n \geq 10$.

the largest path is $P_T(a, d)$: for leaf b it must be:

$$d_T(f, b) \leq \max \{d_T(a, b), d_T(d, b)\}$$

while from the tri-coloring $d_T(a, b), d_T(d, b) \leq d_{max} < d_T(f, b)$.

the largest path is $P_T(a, f)$: for leaf c it must be:

$$d_T(d, c) \leq \max \{d_T(a, c), d_T(f, c)\}$$

while from the tri-coloring $d_T(a, c), d_T(f, c) < d_{min} \leq d_T(d, c)$.

the largest path is $P_T(d, f)$: for leaf e it must be:

$$d_T(a, c) \leq \max \{d_T(d, c), d_T(f, c)\}$$

while from the tri-coloring $d_T(d, c), d_T(f, c) \leq d_{max} < d_T(a, c)$.

In all the three cases, a contradiction arises. □

3.2 Graph C_n^2, $n \geq 8$, is not PCG

We recall that all graphs with at most 7 nodes are PCG [5] and that cycles are PCGs [13], so we focus on $n \geq 8$.

For easing the proofs, the nodes of C_n^2 will be indexed with values in the finite group $\mathbb{Z}_n$ of the integers modulo n, i.e. $V(C_n^2) = \{v_0, v_1, \ldots, v_{n-1}\}$. As a consequence, for each pair v_i, v_j, the edge (v_i, v_j) belongs to C_n^2 if and only if $j - i \in \{1, 2, n-1, n-2\}$.

Before proving that C_n^2 is not PCG, we need some *ad-hoc* forbidden PCG-colorings for C_n^2. Due to the lack of space, we omit the proof, that can be found in [1].

Given a PCG-coloring of C_n^2, we call *red-node* a node v of C_n^2 if all the non-edges incident on v are of red color.

Lemma 7. *Let C_n^2, $n \geq 8$, be a square cycle. Then:*

1. *Any PCG-coloring of C_n^2 where all the 2-non-edges are blue is forbidden.*
2. *Any PCG-coloring of C_n^2 having two red non-edges from a common non red-node to two adjacent nodes is forbidden.*
3. *Any PCG-coloring of C_n^2 having two adjacent red-nodes is forbidden.*

Now we show other two *ad-hoc* forbidden PCG-colorings that hold only for $n \geq 10$ because in the proof we exploit $\mathbf{f}-\mathbf{c}(C)$. Hence the two cases $n=8$ and $n=9$ have to be handled separately. Due to the lack of space, their proof are omitted in this extended abstract and can be found in [1].

Lemma 8. *Let C_n^2, $n \geq 10$, be a square cycle. Then:*

1. *Any PCG-coloring of C_n^2 with a triple of nodes (v_i, v_{i+4}, v_{i+8}), $0 \leq i < n$, such that v_{i+8} is the only non red-node (in this triple) is forbidden.*
2. *Any PCG-coloring of C_n^2 with a triple of nodes (v_{i-6}, v_{i-3}, v_i), $0 \leq i < n$, such that v_{i-6} is the only non red-node (in this triple) is forbidden.*

We are now ready to prove that C_n^2 is not PCG.

Theorem 1. *Graph C_n^2, $n \geq 10$, is not a PCG.*

Proof. The proof is by contradiction. Let (v_i, v_{i+4}) be a red 2-non-edge in C_n^2 (such a non-edge must exist by Lemma 7.1). Consider now the induced path $G[v_i, v_{i+1}, v_{i+3}, v_{i+4}]$. In this path we have the red non-edge (v_i, v_{i+4}) thus, due to $\mathbf{f}-\mathbf{c}(P_4)$, one of the non-edges (v_i, v_{i+3}) and (v_{i+1}, v_{i+4}) is red, too and at least one of the nodes v_i and v_{i+4} is the end-point of two red non-edges toward adjacent nodes. Hence one of these nodes is a red-node (see Lemma 7.2). Reindexing the nodes of C_n^2, this red-node is node v_0.
Consider now the induced subgraph $G[v_{n-3}, v_{n-1}, v_0, v_1, v_2, v_4]$. In this subgraph the non-edges (v_{n-3}, v_0) and (v_0, v_4) are red and, due to $\mathbf{f}-\mathbf{c}(C)$, at least one of the non-edges (v_{n-3}, v_1) and (v_1, v_4) is red. We consider two cases:

non-edge (v_1, v_4) is red

The two non-edges (v_0, v_4) and (v_1, v_4) are red so, by Lemma 7.2, node v_4 is a red-node. Considering the triple of nodes (v_0, v_4, v_8), by Lemma 8.1, node v_8 is a red-node, too. We can iterate this reasoning on the triple (v_4, v_8, v_{12}) and so on, and finally obtaining that $V^* = \{v_i \mid i \equiv 0 \pmod 4\}$ is a set of red-nodes in the PCG-coloring. Moreover each node v_i, with $i \not\equiv 0 \pmod 4$, is adjacent to some node in V^* thus, by Lemma 7.3, n is a multiple of 4 (and $n \geq 12$) and set V^* contains all the red-nodes of the PCG-coloring. Consider now the cycle induced by all the nodes having an odd index, i.e. $G[v_1, v_3, v_5, \ldots, v_{n-1}]$. This cycle is $\frac{n}{2} \geq 6$ long thus, by Lemma 4, it contains at least a red non-edge. Let (v_i, v_j) be one of these red non-edges. Node v_j is necessarily adjacent to a node in V^*, hence there are two red non-edges from adjacent nodes incident toward v_i in C_n^2 implying that v_i is a red-node (by Lemma 7.2). This contradicts the fact that $v_i \notin V^*$.

non-edge (v_{n-3}, v_1) is red

The proof is analogous to the previous one: due to the two red non-edges (v_{n-3}, v_0) and (v_{n-3}, v_1), by Lemma 7.2, node v_{n-3} is a red-node. Considering the triple of nodes (v_{n-6}, v_{n-3}, v_0) in Lemma 8.2, node v_{n-6} is a red-node, too. We can iterate this reasoning on the triple $(v_{n-9}, v_{n-6}, v_{n-3})$ and so on finally obtaining that $V^* = \{v_i \mid i \equiv 0 \pmod 3\}$ is a set of red-nodes in the PCG-coloring. Moreover, each node v_i, with $i \not\equiv 0 \pmod 3$, is adjacent to some node in V^* so, due to Lemma 7.3, n is a multiple of 3 (and $n \geq 12$) and set V^* contains all the red-nodes of the PCG-coloring. Consider now the cycle induced by all the nodes that are not in V^*, i.e. $G[1, 2, 4, \ldots, n-2, n-1]$. This cycle has length at least 8 and, by Lemma 4, there is at least a red non-edge connecting two nodes of the cycle. Let (v_i, v_j) be one of these red non-edges. Node v_j is adjacent to a node in V^*, so v_i is the end-point of two red non-edges toward adjacent nodes in C_n^2 as a consequence v_i is a red-node (by Lemma 7.2). This contradicts the fact that $v_i \notin V^*$. □

Theorem 2. *Graph C_8^2 is not a PCG.*

Corollary 1. *Graph C_8^2 is the smallest planar graph that is not PCG.*

Theorem 3. *Graph C_9^2 is not a PCG.*

3.3 Graph $C_n^2, n \geq 8$, is a minimal graph that is not PCG

Recall that if a graph contains as induced subgraph a not PCG, then it is not PCG, too. We call *minimal not PCG* a graph that is not PCG and it does not contain any induced proper subgraph that is not PCG. (It is worth to be noted that PCG is closed under taking induced subgraphs.)

In this subsection we prove that C_n^2 is a minimal not PCG. The proof is constructive and it provides an edge-weighted tree T and two values d_{min} and d_{max} such that $PCG(T, d_{min}, d_{max}) = C_n^2 \setminus \{x\}$ for any node x of C_n^2.

Theorem 4. *C_n^2, $n \geq 8$, is a minimal not PCG.*

Proof. Consider the graph C_n^2, $n \geq 8$. To prove the theorem we remove from the graph a node x and prove that the new graph G' is PCG. Without loss of generality assume that $x = v_n$. We construct a tree T such that $G' = \text{PCG}(T, 2n-2, 2n+4)$. We consider the following two cases depending on whether n is an even or an odd number.

- *n is an odd number.* Tree T is a caterpillar with $n-1$ internal nodes we denote as $x_1, x_2, \ldots, x_{\frac{n-1}{2}-1}, y, x_{\frac{n-1}{2}}, \ldots, x_{n-2}$. The internal nodes induce a path from x_1 to x_{n-2} and edges (x_i, x_{i+1}), $1 \leq i < (n-1)/2 - 1$ and $(n-1)/2 \leq i < n-2$, have weight 2. Edges $(x_{\frac{n-1}{2}-1}, y)$ and $(y, x_{\frac{n-1}{2}})$ have weight 1. Leaves v_i, $1 \leq i \leq n-2$, are connected to x_i with edges of weight n. Finally leaf v_{n-1} is connected to the node y with an edge of weight 3. See Figure 4.a
- *n is an even number.* Tree T is a caterpillar with $n-1$ internal nodes we denote as $x_1, x_2, \ldots, x_{n-1}$. The internal nodes $x_1, \ldots, x_{n-1}$ induce a path and edges (x_i, x_{i+1}), $1 \leq i < n-1$, have weight 2.

Leaves v_i, $1 \leq i < n$, are connected to x_i with edges of weight n. Finally v_{n-1} is connected to $x_{\frac{n-2}{2}}$ with an edge of weight 3. See Figure 4.b. □

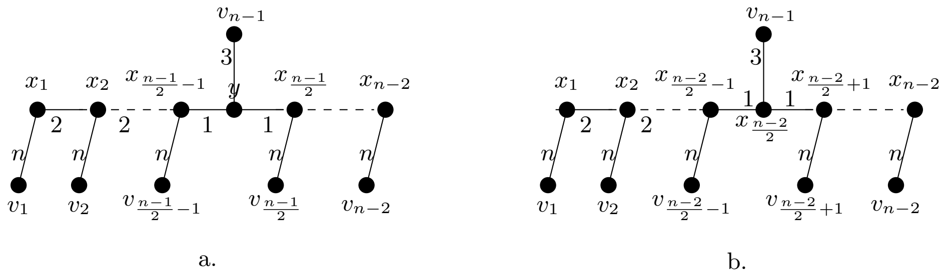


Fig. 4. Caterpillars for the proof of Theorem 4: a. n odd; b. n even.

4 Other results due to the application of our technique

In this section we get two further results applying again the technique introduced in Section 2. Due to the lack of space, we omit the proofs, that can although be found in [1]. The graph classes we consider are obtained by operating in different ways on cycles and are very interesting in this context because both are connected to some open problems.

4.1 The wheel

Wheels W_{n+1} are n length cycles C_n whose nodes are all connected with a universal node.

Wheel W_{6+1} is PCG and it is the only graph with 7 nodes whose witness tree is not a caterpillar [5]. Moreover, it has been proven in [4] that also the larger wheels up to W_{10+1} do not have a caterpillar as a witness tree but, up to now, no other witness trees are known for these graphs and, in general, it has been left open to understand whether wheels with at least 8 nodes are PCGs or not.

Using our technique, we prove the following theorem.

Theorem 5. *Wheel W_{7+1} is a PCG while wheels W_{n+1}, $n \geq 8$, are minimal not PCGs.*

4.2 The strong product of a cycle and P_2

Given two graphs G and H, their *strong product* $G\Box H$ is a graph whose node set is the cartesian product of the node sets of the two graphs, and there is an edge between nodes (u, v) and (u', v') if and only if either $u = u'$ and (v, v') is an edge of H or $v = v'$ and (u, u') is an edge of G.

We recall that $C_4\Box P_2$ has already been proved not to be PCG [8] but nothing is known for $n > 4$. Recalling that all graphs with 7 nodes or less are PCGs, our result is the following.

Theorem 6. *The graphs obtained as strong product $C_n\Box P_2$, $n \geq 4$ are minimal not PCGs.*

5 Conclusions

In this paper we proposed a new proof technique to show that graphs are not PCGs. As an example, we applied it to the square of cycles, to wheels and to $C_n \square P_2$. As a side effect, we show that the smallest planar graph not to be PCG has not 20 nodes, as previously known, but only 8.

Even if all these classes are obtained by operating on cycles, we think that this technique can be potentially used to position outside PCG many other graph classes no related to cycles. This represents an important step toward the solution of the very general open problem consisting in demarcating the boundary of the PCG class.

References

1. P.Baiocchi, T. Calamoneri, A. Monti, R. Petreschi. Some classes of graphs that are not PCGs. arXiv:1707.07436 [cs.DM].
2. A. Brandstädt. On Leaf Powers. *Technical report*, University of Rostock, 2010.
3. A. Brandstädt, C. Hundt. Ptolemaic graphs and interval graphs are leaf powers. Proc. *Theoretical Informatics (LATIN)*, Lecture Notes in Computer Science 4957, 479–491, 2008.
4. T. Calamoneri, A. Frangioni, B. Sinaimeri. Pairwise Compatibility Graphs of Caterpillars. *The Computer Journal* **57(11)** 1616–1623, 2014.
5. T. Calamoneri, D. Frascaria, B. Sinaimeri. All graphs with at most seven vertices are Pairwise Compatibility Graphs. *The Computer Journal* **56(7)** 882-886, 2013.
6. T. Calamoneri, B. Sinaimeri. On Pairwise Compatibility Graphs: a Survey. *SIAM Review* **58(3)** 445-460, 2016.
7. T. Calamoneri, R. Petreschi. On pairwise compatibility graphs having Dilworth number two. *Theoretical Computer Science* **524** 34–40, 2014.
8. S. Durocher, D. Mondal, Md. S. Rahman. On graphs that are not PCGs. *Theoretical Computer Science* **571** 78–87, 2015.
9. J. Felsenstein. Cases in which parsimony or compatibility methods will be positively misleading. *Systematic Zoology*, **27**, 401–410, 1978.
10. P.E. Kearney, J. I. Munro, D. Phillips. Efficient generation of uniform samples from phylogenetic trees. Proc. *Algorithms in Bioinformatics*, Lecture Notes in Computer Science 2812, 177–189, 2003.
11. S. Mehnaz and M.S. Rahman. Pairwise compatibility graphs revisited. Proc. *International Conference on Informatics, Electronics Vision (ICIEV)*, 2013.
12. S.A. Salma, Md. S. Rahman. Triangle-Free Outerplanar 3-Graphs are Pairwise Compatibility Graphs. *J. Graph Algorithms Appl.*, **17(2)** 81–102, 2013.
13. M.N. Yanhaona, Md.S. Bayzid, Md. S. Rahman. Discovering Pairwise Compatibility Graphs. *Discrete Mathematics, Algorithms and Applications*, **2(4)**, 607–623, 2010.
14. M.N. Yanhaona, K.S.M.T. Hossain, Md. S. Rahman. Pairwise Compatibility Graphs. *Journal of Applied Mathematics and Computing*, **30**, 479–503, 2009.
15. Md. I. Hossain, S.A. Salma, Md. S. Rahman, D. Mondal: A Necessary Condition and a Sufficient Condition for Pairwise Compatibility Graphs. *J. Graph Algorithms Appl.*, **21(3)** 341–352, 2017.