Some classes of graphs that are not Pairwise Compatibility Graphs (Communication)

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1 Introduction

Graphs we deal with in this paper are motivated by a fundamental problem in computational biology, that is the reconstruction of phylogenetic trees, i.e. trees where leaves represent known taxa while internal nodes possible ancestors that might have led through evolution to this set of taxa [8]. The tree reconstruction problem is proved to be NP-hard under many criteria of optimality, moreover real phylogenetic trees are usually huge, so testing possible 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 biologicallymotivated constraints, and to test the reconstruction algorithms only on the smaller subtrees induced by the sample. Using in the sample very close or very distant taxa can create problems for phylogeny reconstruction algorithms [5] so, in selecting a sample from the leaves of the tree, the constraint of keeping the pairwise 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 (PCGs).

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. In such a case, we say that G is a PCG of T for d_{min} and d_{max} ; in symbols, $G = PCG(T, d_{min}, d_{max})$ [3,6].



Fig. 1. a. A graph G. b. An edge-weighted caterpillar T such that G = PCG(T, 4, 5).

In Figure 1.a a small graph that is PCG(T, 4, 5) is depicted and, in Figure 1.b, T is shown. In general, T is not unique; here T is a *caterpillar*, i.e. a tree consisting of a central path to which all the other nodes are directly connected. 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 [2].

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 [6]. This conjecture has been confuted by proving the existence of some graphs not belonging to PCG. Namely, Yanhaona et al. [9] show a not PCG bipartite graph with 15 nodes (Figure 2.a). More recently, Durochet et al. [4] prove that there exists a not bipartite graph with 8 nodes that is not PCG (Figure 2.b); this is the smallest graph that is not PCG, since all graphs with at most 7 nodes are PCGs [2]. Subsequently, Mehnaz and Rahman [7] generalize the technique in [9] to provide a class of bipartite graphs that are not PCGs. The authors of [4] provide also an example of a planar graph with 20 nodes that is not a PCG (Figure 2.c).

It remains unclear which is the boundary between PCGs and not PCGs, so we focus on searching new graph classes that are not PCGs.



Fig. 2. a. The first graph proven not to be a PCG. b. The graph of smallest size proven not to be a PCG. c. A planar graph that is not PCG.

Namely, we consider three classes of *n*-node graphs, $n \ge 8$, that are all modifications of cycles:

- graphs obtained as strong product between an n/2 cycle and K_2 ;
- graphs obtained as the square of an n cycle;
- graphs obtained connecting the nodes of an (n-1) cycle with an universal node (wheels).

We study the first class because naturally extends the graph in Figure 2.b, that can be interpreted as $C_4 \Box K_2$. The graphs in the second class are a natural variation of cycles, that have been proved to be PCGs [10]. Finally, we deep inside the wheels as they have already been studied from the pairwise compatibility point of view. Indeed, wheel W_7 is PCG and it is the only graph with 7 nodes whose witness tree is not a caterpillar [2] (see Figure 3.a). Moreover, it has been proven in [1] that also the larger wheels up to W_{11} 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.

In the following section we communicate all our results concerning these three classes in relation to the pairwise compatibility property. All the proofs are detailed in the extended version of this paper.

2 Results

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



Fig. 3. a. Tree *T* such that $W_7 = PCG(T, 5, 7)$; b. Tree *T* such that $W_8 = PCG(T, 9, 13)$.

only if either u = u' and (v, v') is an edge of H or v = v' and (u, u') is an edge of G or both (u, u') and (v, v') are edges in G and H respectively.

Theorem 1. Let $k \ge 4$. The graph $C_k \Box K_2$ is not PCG.

We highlight that when k = 4, $C_k \Box K_2$ is the graph in Figure 2.b and it is known not to be PCG. In the extended version of this paper we present an *ad-hoc* proof for k = 5 and a general proof for $k \ge 6$.

Given a graph G, its square graph G^2 is a graph whose node set coincides with the node set of G and there is an edge (u, v) in G^2 if and only if either u and v are adjacent or they are connected by a 2 length path in G.

Theorem 2. Let $n \ge 8$. The square of cycle C_n is not PCG.

Also in this case, we prove separately the cases n = 8, 9 from the general case $n \ge 10$.

Let W_n be the *wheel* obtained by connecting all the nodes of an (n-1) cycle C_{n-1} with a central (universal) node.

It is known that W_7 is PCG (see a witness tree in Figure 3.a). In Figure 3.b we show a witness tree for W_8 , so proving the following theorem:

Theorem 3. Wheel W_8 is PCG.

On the contrary, when $n \ge 8$, we prove that wheels are not PCGs:

Theorem 4. Let $n \ge 9$. The graph W_n is not PCG.

Our last results concern minimality of the previously defined classes of graphs, where a not PCG is *minimal* if, by deleting any node from it, we get a PCG.

Theorem 5. Let $k \ge 4$. The graph obtained by removing any node from $C_k \Box K_2$ is PCG. In other words, $C_k \Box K_2$ is a minimal not PCG.

Theorem 6. Let $k \ge 4$. The graph obtained by removing any node from C^2 is PCG. In other words, C^2 is a minimal not PCG.

Theorem 7. Let $n \ge 9$. The graph obtained by removing any node from W_n is PCG. In other words, W_n is a minimal not PCG.

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