Pairwise Compatibility Graphs
(Invited Talk)

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Abstract. Pairwise Compatibility Graphs (PCG) are graphs introduced in relation to the biological problem of reconstructing phylogenetic trees. Without demanding to be exhaustive, in this note we take a quick look at what is known in the literature for these graphs.

The evolutionary history of a set of organisms is usually represented by a tree-like structure called *phylogenetic tree*, where the leaves are the known species and the internal nodes are the possible ancestors that might have led, through evolution, to this set of species. Edges are evolutionary relationships between species, while the edge weights represent evolutionary distances among species (evolutionary times).
The *phylogenetic tree reconstruction problem* consists in finding a fully labeled phylogenetic tree that 'best' explains the evolution of given species, where 'best' means that it optimizes a specific target function.
Tree reconstruction problem is proved to be NP-hard under many criteria of optimality, so the performance of the heuristics for this problem is usually experimentally evaluated by comparing the output trees with the partial trees that are unanimously recognized as sure by biologists. But real data consist of a huge number of species, and it is unfeasible to compare trees with such a number of leaves, so it is common to exploit sample techniques. The idea is to find efficient ways to sample subsets of species from a large set in order to test the heuristics on the smaller sub-trees induced by the sample. The constraints on the sample attempt to ensure that the behavior of the heuristics will not be biased by the fact it is applied on the sample instead of on the whole tree. Since very close or very distant taxa can create problems for phylogenetic reconstruction heuristics [9], the following definition of Pairwise Compatibility Graphs [12] appears natural:

Definition 1. *Graph* $G = (V, E)$ *is a* Pairwise Compatibility Graph, $PCG(T, d_{min}, d_{max})$*, if:*
$V = Leaves(T)$ *and* $E = \{(u, v) | d_{min} \leq d_{T(u,v)} \leq d_{max}\}$ *where:*
- T *is a positive edge-weighted tree and is called* witness tree for G*;*
- $d_{T(u,v)}$ *is the sum of the weights of all the edges on the (unique) path from* u *to* v *on* T*;*
- d_{min} *and* d_{max} *are two nonnegative values.*

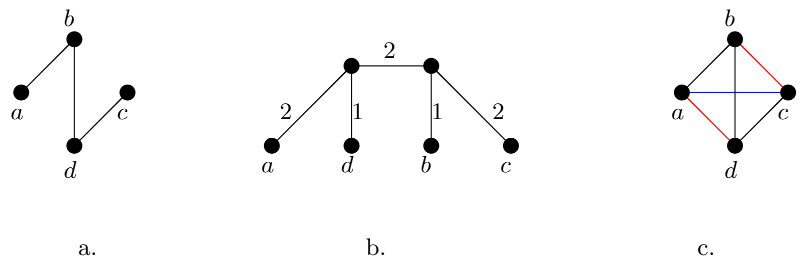

Fig. 1. a. A graph G. b. An edge-weighted tree T such that $G = PCG(T, 4, 5)$. c. The PCG-coloring induced on G by triple $T, 4, 5$.

In fig. 1.a graph $G = PCG(T, 4, 5)$ is depicted, where T is shown in fig. 1.b.
The sample problem in terms of graph theory is hence strictly related with the *PCG recognition problem*, asking whether a given graph is PCG, for some tree T and values d_{min} and d_{max}. While it is trivial to construct graph G starting from T, d_{min}, d_{max}, the inverse problem is difficult and it has been conjectured that this problem is NP-hard, so the aim of the researchers has been to prove or disprove the conjecture; to this aim, some graph classes have been proved to be inside and outside PCGs, moreover some steps towards characterization of PCGs have been done (conditions, techniques, properties, ...).

In the following we will present a brief overview of some results on PCGs.

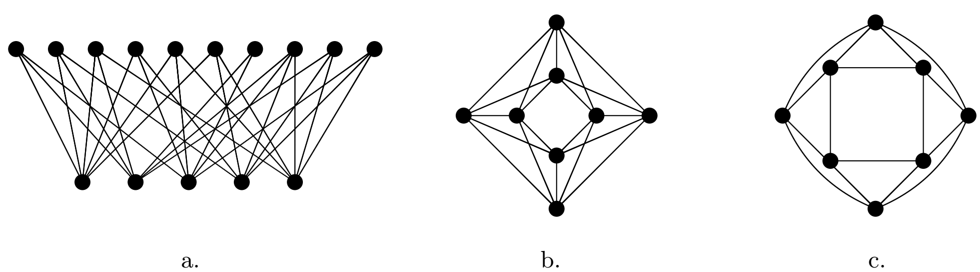

Fig. 2. a. The first graph proven not to be a PCG. b. The (not planar) graph of smallest size proven not to be a PCG. c. The (planar) graph of smallest size proven not to be a PCG.

It was conjectured [12] that all graphs are PCGs, but this was disproved in 2010 showing that the graph in Fig. 2.a cannot be PCG [16].
All graphs with a number of nodes not greater than 7 are PCGs [3] and there are examples of graphs with 8 nodes that are not PCGs (see Fig.2.b [8] and 2.c [1]).

Some classes of graphs are pairwise compatibility; among them there are interval graphs [2], cliques, trees,cycles, cacti, single chord cycles [16, 17], triangle-free outerplanar 3-graphs [15], subclasses of split matrogenic graphs [5].
Moreover some classes of graphs are not pairwise compatibility, such as some bipartite graphs [16], tolerance graphs [4], permutation graphs [7], graphs that are the strong product between C_n and P_2, $n > 4$ [1] and the square of a cycle [1].

Since all graphs with 7 vertices are PCGs, it is natural to wonder whether some interesting classes of graphs remain PCGs or not when they have $n \geq 8$ nodes. The n node wheels W_n behave in an unexpected way: wheel with 7 nodes, W_7, is clearly PCG (see Fig. 3.a for a witness tree [3]); wheel with 8 nodes has later been proved to be also in PCG (see Fig. 3.b for a witness tree) while larger wheels (with 9 or more nodes) are not PCGs anymore [1].

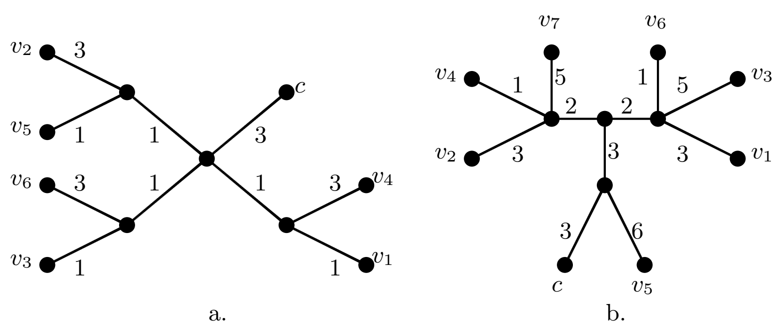

Fig. 3. a. Tree T such that $W_7 = PCG(T, 5, 7)$; b. Tree T such that $W_8 = PCG(T, 9, 13)$.

The following results are not restricted to special classes of graphs and are mainly based on the definition of tri-coloring:

Definition 2. *[1] A* tri-coloring *C is an edge-coloring of a $PCG(T, d_{min}, d_{max})$ such that:*
- *(u, v) is red in C if $d(u, v) < d_{min}$,*
- *(u, v) is black in C if $d_{min} \leq d(u, v) \leq d_{max}$,*
- *(u, v) is blue in C if $d(u, v) > d_{max}$.*

We say that triple (T, d_{min}, d_{max}) induces *C.*

In fig. 1.c a tri-coloring for the graph of fig. 1.a is depicted.
A tri-coloring C (even only partial) of a graph G is *forbidden* if no triple (T, d_{min}, d_{max}) inducing C exists.
It holds that:

- Any induced subgraph H of a given PCG G inherits the tri-coloring C of G and so is PCG, too (easy to prove).
- If a graph contains as induced subgraph a not PCG, then it is not PCG, too (easy to prove by contradiction).

– If a tri-coloring C of a graph G is forbidden for a PCG subgraph of G, then it is forbidden also for G. Consequently, G is not PCG if and only if each tri-coloring of a graph G induces a forbidden tri-coloring in at least an induced PCG subgraph of G [1].
– Let G be a graph and let G^c be its complement. If G^c has two disjoint chordless cycles, then G is not a PCG. If G^c has no cycles, then G is a PCG [11]
– A graph G consisting of two graphs $G_1$and G_2 that share a node as a cut-node in G is a PCG if and only if both G_1 and G_2 are PCG [18].

In Fig. 4 an interesting picture shows how PCGs contain many well known classes of graphs. Here there are the definitions of all the named subclasses:

– $\mathcal{C}$: cycles;
– LPG: Leaf Power Graphs, i.e. PCGs in which d_{min} is always equal to 0: $G = PCG(T, 0, d_{max}) = LPG(T, d_{max})$ [2, 14];
– $mLPG$: Minimum Leaf Power Graphs, i.e. PCGs in which d_{max} is always equal to ∞: $G = mLPG(T, d_{min}) = PCG(T, d_{min}, \infty)$ [6];
– $\mathcal{T}$: threshold graphs, i.e. split graphs with the neighborhoods of the vertices nested [10];
– $\mathcal{SM}$: Split Matching graphs, i.e. split graphs where the subgraph connecting the clique and the stable set is a perfect mathching [13];
– $\mathcal{SA}$: Split Anti-matching graphs, i.e. split graphs where the subgraph connecting the clique and the stable set is a perfect anti-mathching [13].

It holds that the complement of every graph in LPG is in mLPG and, conversely, the complement of every graph in mLPG is in LPG [5]. It would be interesting to understand which other graph classes are in PCG and in particular to study if threshold graphs are the only graphs in the intersection between LPG and mLPG or not.

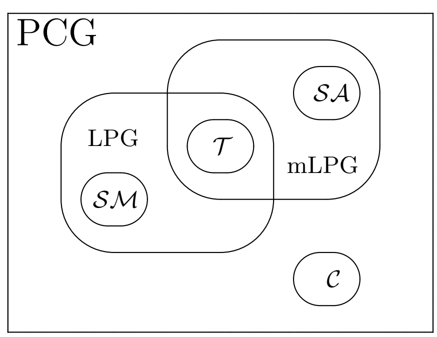

Fig. 4. Relationships between PCG and other interesting classes of graphs [6].

To conclude this brief presentation on PCGs, we make some considerations on different classes of trees that can be witness trees of a PCG.

Caterpillars and stars are very simple and natural tree structures so, since PCGs may have different witness trees, they have often been exploited to prove that some graph classes are in PCG. Nevertheless there are graphs that are PCGs, but not PCGs of caterpillars nor of stars. Consequently, it appears very natural to characterize PCGs that have as witness tree one of these two tree structures. For what concerns caterpillars, the complete characterization of PCGs of caterpillars is at moment an interesting open problem since the literature contains results only on caterpillars with all weights equal 1. Namely,it is known that graph classes $PCG(T, 0, d_{max})$ and unit interval graphs are equivalent when T is a caterpillar with all weights equal 1 [2]. In [3] this result has been generalized to any value of d_{min}. For what it concerns stars, it is known that PCGs of stars are a superclass of threshold graphs; indeed, it is possible to partition the nodes of a PCG of a star in such a way that one partition induces a clique, while the other two induce two stable sets, where the subclasses induced by the clique and each one of the stable sets are threshold graphs (see fig. 5) [6].
It is worth to be noticed that there exists an algorithm requiring $O(n^6)$ time for testing if a given n node graph is PCG of a star or not [19].

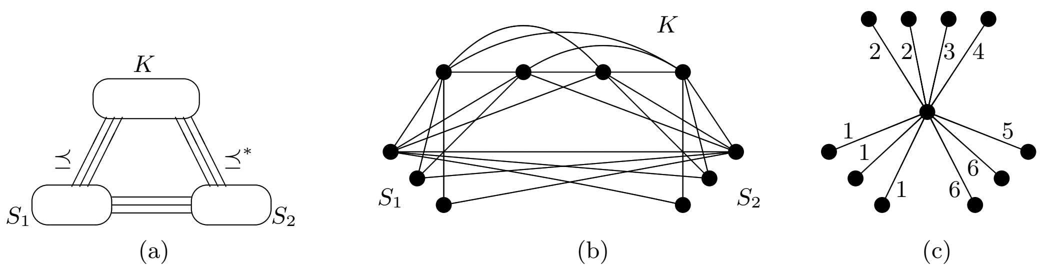

Fig. 5. (a) The structure of a PCG generated by a star; (b) the PCG generated by the star depicted in (c).

References

1. P. Baiocchi, T. Calamoneri, A. Monti, R. Petreschi (2018) Graphs that are Not Pairwise Compatible: A New Proof Technique (Extended Abstract), Proc. IWOCA 2018, Lecture Notes in Computer Science, in press. Also presented at ICTCS 2017, CEUR Workshop Proceedings 1949, 203–207.
2. A. Brandstädt, C. Hundt (2008) Ptolemaic graphs and interval graphs are leaf powers, Proc. LATIN 2008, Lecture Notes in Comput. Sci. 4957, pp. 479–491.

3. T. Calamoneri, D. Frascaria, B. Sinaimeri (2014) All graphs with at most seven vertices are Pairwise Compatibility Graphs, The Computer Journal 56(7) 882–886.
4. T. Calamoneri, M. Gastaldello, B. Sinaimeri (2015) On Pairwise Compatibility of Some Graph (Super)classes, arXiv:1504.06454.
5. T. Calamoneri, E. Montefusco, R. Petreschi, B. Sinaimeri (2013) Exploring pairwise compatibility graphs, Theoret. Comput. Sci., 468 23–26.
6. T. Calamoneri, R. Petreschi, B. Sinaimeri (2013) Pairwise compatibility property of some superclasses of threshold graphs, Discrete Math. Algorithms Appl., 5.
7. T. Calamoneri, B. Sinaimeri (2016) On Pairwise Compatibility Graphs: a Survey. SIAM Review 58(3) 445–460.
8. S. Durocher, D. Mondal, Md. S. Ramhan (2015) On graphs that are not PCGs, Theoretical Computer Science 571 78–87.
9. J. Felsenstein (1978) Cases in which parsimony or compatibility methods will be positively misleading, Systematic Zoology, 27 401–410.
10. V. Chvátal, P. Hammer (1977) Aggregation of inequalities in integer programming, Annals of Discrete Mathematics, 1 145–162.
11. Md.I. Hossain, S. A. Salma, Md. S. Rahman, D. Mondal (2017) A Necessary Condition and a Sufficient Condition for Pairwise Compatibility Graphs, J. Graph Algorithms Appl. 21(3) 341–352.
12. P.E. Kearney, J. I. Munro, D. Phillips (2003) Efficient generation of uniform samples from phylogenetic trees, Proc. *Algorithms in Bioinformatics*, Lecture Notes in Computer Science 2812 177–189.
13. N. Mahadev, U. Peled (1995) Threshold graphs and related topics, Annals of Discrete Mathematics 56.
14. N. Nishimura, P. Ragde, D.M. Thilikos (2002) On graph powers for leaf-labeled trees, Journal of Algorithms 42 (1) 69–108.
15. S. A. Salma, Md. S. Rahman, Md. I. Hossain (2013) Triangle-free outerplanar 3-graphs are pairwise compatibility graphs, J. Graph Algorithms Appl., 17 81–102.
16. M.N. Yanhaona, Md.S. Bayzid, Md. S. Rahman (2010) Discovering Pairwise Compatibility Graphs, Discrete Mathematics, Algorithms and Applications 2(4) 607–623.
17. M. N. Yanhaona, K. S. M. T. Hossain, Md. S. Rahman (2009) Pairwise compatibility graphs, J. Appl. Math. Comput., 30 479–503.
18. M. Xiao, H. Nagamochi (2018) Some reduction operations to pairwise compatibility graphs, arXiv: 1804.02887v1//9Apr
19. M. Xiao, H. Nagamochi (2018) Characterizing Star-PCGs, arXiv: 1804.02895v1//9Apr