A SHORT NOTE ON UNDIRECTED FITCH GRAPHS

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ABSTRACT. The symmetric version of Fitch’s xenology relation coincides with class of complete multipartite graph and thus cannot convey any non-trivial phylogenetic information.

Fitch graphs [4] form a class of directed graphs that is derived from rooted, \{0,1\}-edge-labeled trees \(T\) in the following manner: The vertices of the Fitch graph are the leaves of \(T\). Two distinct leaves \(x\) and \(y\) of \(T\) are connected by an arc \((x, y)\) from \(x\) to \(y\) if and only if there is at least one edge with label 1 on the (unique) path in \(T\) that connects the least common ancestor \(\text{lca}(x, y)\) of \(x\) and \(y\) with \(y\). Fitch graphs model “xenology”, an important binary relation among genes introduced by Walter M. Fitch [2]. Interpreting \(T\) as a phylogenetic tree and 1-edges as horizontal gene transfer events, the arc \((x, y)\) in the Fitch graph encodes the fact that \(y\) is xenologous with respect to \(x\). The directed Fitch graphs are the topic of Ref. [4], which among other results proves a characterization in terms of eight forbidden induced subgraphs.

It is natural to consider the symmetrized version of this relationship, i.e., to interpret \(\{x, y\}\) as a xenologous pair whenever the evolutionary history separated \(x\) and \(y\) by at least one horizontal transfer event. In mathematical terms, this idea is captured by

\textbf{Definition 1.} Let \(T\) be a rooted tree with leaf set \(X\) and let \(\lambda : E(T) \to \{0, 1\}\). Then the undirected Fitch graph \(F\) explained by \((T, \lambda)\) has vertex set \(X\) and edges \(\{x, y\} \in E(F)\) if and only if there is a path in \(T\) from \(x\) to \(y\) containing at least one edge \(e\) with \(\lambda(e) = 1\). A graph \(F\) is an undirected Fitch graph if and only if it is explained in this manner by some edge-labeled rooted tree \((T, \lambda)\).

Undirected Fitch graphs are closely related to their directed counterparts. Since the path \(\rho\) connecting two leaves \(x\) and \(y\) is unique and contains their last common ancestor \(\text{lca}(x, y)\), there is a 1-edge along \(\rho\) if and only if there is 1-edge on the path between \(x\) and \(y\) or between \(\text{lca}(x, y)\) and \(y\). The undirected Fitch graph is therefore the underlying undirected graph of the directed Fitch graph, i.e., it is obtained from the directed version by ignoring the direction of the arcs.

The undirected Fitch graphs form a heritable family, i.e., if \(F\) is an undirected Fitch graph, so are all its induced subgraphs. This is an immediate consequence of the fact that directed Fitch graphs are a heritable family of digraphs [4]. The fact can also be obtained directly by considering the restriction of \(T\) to a subset of leaves. This obviously does not affect the paths or their labeling between the remaining vertices.

Clearly \(F\) does not depend on which of the non-leaf vertices in \(T\) is the root. Furthermore, a vertex \(v\) with only two neighbors and its two incident edges \(e'\) and \(e''\) can be replaced by a single edge \(e\). The new edge is labeled \(\lambda(e) = 0\) if both \(\lambda(e') = \lambda(e'') = 0\), and \(\lambda(e) = 1\) otherwise. These operations do not affect the undirected Fitch graph. Hence, we can replace the rooted tree \(T\) by an unrooted tree in Def. 1 and assume that all non-leaf edges have at least degree 3. To avoid trivial cases we assume throughout that \(T\) has at least two leaves and hence a Fitch graph has at least two vertices.

\textbf{Lemma 1.} If \(G\) is an undirected Fitch graph, then \(G\) does not contain \(K_1 \cup K_2\) as an induced subgraph. In particular every undirected Fitch graph is a complete multipartite graph.

\textbf{Date:} December 6, 2017.

1991 \textit{Mathematics Subject Classification.} 05C75, 05C05, 92B10.

\textit{Key words and phrases.} Labeled trees, forbidden subgraphs, phylogenetics, xenology, Fitch graph.

This work is supported in part by the BMBF-funded project “Center for RNA-Bioinformatics” (031A538A, de.NBI/RBC).
Theorem 1. There is a single unrooted tree with three leaves, namely the star $S_3$, which admits four non-isomorphic $\{0, 1\}$-edge labelings defined by the number $N$ of 1-edges. The undirected Fitch graphs $F_N$ are easily obtained. In the absence of 1-edges, $F_0 = K_3$ is edge-less. For $N = 2$ and $N = 3$ there is 1-edge along the path between any two leaves, i.e., $F_2 = F_3 = K_3$. For $N = 1$ one leaf is connected to the other two by a path in $S_3$ with an 1-edge; the path between the latter two leaves consists of two 0-edges, hence $F_1 = P_3$, the path of length two. Hence, only three of the four possible undirected graphs on three vertices can be realized, while $K_1 \cup K_2$ is not an undirected Fitch graph. By heredity, $K_1 \cup K_2$ is therefore a forbidden induced subgraph for the class of undirected Fitch graphs. Finally, it is well known that the class of graphs that do not contain $K_1 \cup K_2$ as an induced subgraph are exactly the complete multipartite graphs, see e.g. [6].

In order to show that forbidding $K_1 \cup K_2$ is also sufficient, we explicitly construct the edge-labeled trees necessary to explain complete multipartite graphs. We start by recalling that each complete multipartite graph $K_{n_1, \ldots, n_k}$ is determined by its independent sets $V_1, \ldots, V_k$ with $|V_i| = n_i$ for $1 \leq i \leq k$. By definition, $\{x, y\} \in E(K_{n_1, \ldots, n_k})$ if and only if $x \in V_i$ and $y \in V_j$ with $i \neq j$. In particular, therefore, $K_{n_1, \ldots, n_k}$ with at least two vertices is connected if and only if $k \geq 2$. The complete 1-partite graphs are the edge-less graphs $\overline{K_n}$.

Since $K_1 \cup K_2$ is an induced subgraph of the path on four vertices $P_4$, any graph $G$ that does not contain $K_1 \cup K_2$ as an induced subgraph must be $P_4$-free, i.e., a cograph [1]. Cographs are associated with vertex-labeled trees known as cotrees, which in turn are a special case of modular decomposition trees [3]. The cotrees of connected multipartite graphs have a particularly simple shape, illustrated without the vertex labels in Fig. 1. The cotree has a root labeled “1” and all inner vertices labeled “0”. Here we do not need the connection between cographs and their cotrees, however. Therefore we introduce these trees together with an edge-labeling that is useful for our purposes in the following

Definition 2. For $k = 1$, $T[n]$ is the star graph $S_n$ with $n$ leaves. For $k \geq 2$, the tree $T[n_1, \ldots, n_k]$ has a root $r$ with $k$ children $c_i$, $1 \leq i \leq k$. The vertex $c_i$ is a leaf if $|V_i| = n_i = 1$ and has exactly $n_i$ children that are leaves if $|V_i| = n_i \geq 2$. For $k = 1$ all edges $e$ of $T[n]$ are labeled $\lambda^*(e) = 0$. For $k \geq 2$ we set $\lambda^*(\{r, c_i\}) = 1$ for $1 \leq i \leq k$ and $\lambda^*(e) = 0$ for all edges not incident to the root.

Now we can prove our main result:

Theorem 1. A graph $G$ is an undirected Fitch graph if and only if it is a complete multipartite graph. In particular, $K_{n_1, \ldots, n_k}$ is explained by $(T[n_1, \ldots, n_k], \lambda^*)$.

Proof. Lemma 1 implies that an undirected Fitch graph is a complete multipartite graph. To show the converse, we fix an arbitrary complete multipartite graph $G = K_{n_1, \ldots, n_k}$ and find an edge-labeled rooted tree $(T, \lambda^*)$ that explains $G$.

For $k = 1$ it is trivial that $(T[n], \lambda^*)$ explains $\overline{K_n}$.

For $k \geq 2$ consider the tree $T[n_1, \ldots, n_k]$ with edge labeling $\lambda^*$ and let $F$ be the corresponding Fitch graph. The leaf-set of $T[n_1, \ldots, n_k]$ partitioned into exactly $k$ subsets $L_1, \ldots, L_k$ defined by (a) singletons adjacent to the root and (b) subsets comprising at least two leaves adjacent to the same child $c_i$ of the root. Furthermore, we can order the leaf sets so that $|L_i| = n_i$. By construction, all vertices within a leaf set $L_i$ are connected by a path that does not run through the root and thus, contains only 0-edges, if $|L_i| > 1$ and no edge, otherwise. The $L_i$ are independent sets in $F$.
In the context of phylogenetic combinatorics is that the

These trees have the smallest possible number (7) of vertices and thus are minimal. These can be obtained from the tree \((T[2,2,1],\lambda^*)\) specified in Definition 1 by contracting one of its inner 1-edge and possibly re-routing the resulting tree.

On the other any two leaves \(x \in L_i\) and \(y \in L_j\) with \(i \neq j\) are connected only by path through the root, which contains two 1-edges. Thus \(x\) and \(y\) are connected by an edge in \(F\). Thus \(F\) is a complete multipartite graph of the form \(K_{[L_1,..,L_k]} = K_{n_1,..,n_k}\). Since \(K_{n_1,..,n_k}\) is explained by \((T[n_1,..,n_k],\lambda^*)\) for all \(n_i \geq 1\) and \(k \geq 2\), and \(K_n\) is explained by \((T[n],\lambda^*)\), we conclude that every complete multipartite graph is a Fitch graph.

Complete multipartite graphs \(G = (V, E)\) obviously can be recognized in \(O(|V|^2)\) time e.g., by checking that its complement is a disjoint union of complete graphs, and even in \(O(|V| + |E|)\) time by explicitly constructing its modular decomposition tree \([5]\). Given the tree \(T[n_1,..,n_k]\), the canonical edge labeling \(\lambda^*\) is then assigned in \(O(|V|)\) time.

A tree \((T,\lambda)\) that explains a Fitch graph \(F\) is minimum if it has the smallest number of vertices among all trees that explain \(F\). In this case, \((T,\lambda)\) is also least-resolved, i.e., the contraction of any edge in \((T,\lambda)\) results in a tree that does not explain \(F\). Not surprisingly, the tree \(T[n_1,..,n_k]\) is almost minimum in most, and minimum in some cases: Since the vertices of the Fitch graph must correspond to leaves of the tree, \(T[n_1,..,n_k]\) is necessarily minimum whenever it is a star, i.e., for \(T[n]\) and \(T[1,..,1]\). In all other cases, its only potentially “superfluous” part is its root. Indeed, exactly one of the edges connecting the root with a non-leaf neighbor can be contracted without changing the corresponding Fitch graph. It is clear that this graph is minimal: The leaf sets \(L_i\) must be leaves of an induced subtree without an intervening 1-edge. Having all vertices of \(L_i\) adjacent to the same vertex is obviously the minimal choice. Since the \(L_i\) must be separated from all other leaves by a 1-edge, at least one neighbor of \(c_i\) must be a 1-edge. Removing all leaves incident to a 0-edge results in a tree with at least \(k\) vertices that must contain at least \(k-1\) 1-edges, since every path between leaves in this tree must contain a 1-edge. These trees have the smallest possible number (7) of vertices and thus are minimal. These can be obtained from the tree \((T[2,2,1],\lambda^*)\) specified in Definition 1 by contracting one of its inner 1-edge and possibly re-routing the resulting tree.

The practical implication of Thm. 1 in the context of phylogenetic combinatorics is that the mutual xenology relation cannot convey any interesting phylogenetic information: Since the undirected Fitch graphs are exactly the complete multipartite graphs, which in turn are completely defined by their independent sets, the only insight we can gain by considering mutual xenology is the identification of the maximal subsets of taxa that have not experienced any horizontal transfer events among them.

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