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Graphs that have clique (partial) 2-trees

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Much of the theory—and the applicability—of chordal graphs is based on their being the graphs that have clique trees. Chordal graphs can be generalized to the graphs that have clique representations that are 2-trees, or even series-parallel graphs (partial 2-trees) or outerplanar or maximal outerplanar graphs. The resulting graph classes can be characterized by forbidding contractions of a few induced subgraphs. There is also a plausible application of such graphs to systems biology.

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1. Clique graphs and clique trees

For any graph G, define the *clique graph* $K(G)$ to be the intersection graph of the family of all *maxcliques*—inclusion-maximal complete subgraphs—of G; in other words, the nodes of $K(G)$ are the maxcliques of G, with two nodes adjacent in $K(G)$ if and only if the corresponding maxcliques have nonempty intersection. (The vertices of $K(G)$ will be called *nodes* in order to lessen confusion with the vertices of G, and a maxclique subgraph Q will be routinely identified with its vertex set $V(Q)$ for convenience.)

For every graph H that has the maxcliques of G as its nodes and for every $v \in V(G)$, define H_v to be the subgraph of H that is induced by those nodes that contain v. Define a tree T whose nodes are the maxcliques of G to be a *clique tree* for G if each T_v is connected; in other words, each T_v is a subtree of T. (Notice that if G and, therefore, $K(G)$ are not connected, then a clique tree T for G will not be a subgraph of $K(G)$, since T will have at least one edge QQ' with $Q \cap Q' = \emptyset$ that is not allowed in $K(G)$.) Theorem 1.1 will characterize the graphs that have clique trees.

A graph is *chordal* if every induced cycle is a triangle. Theorem 1.1 underlies both much of the theory [10] and many of the applications [9, 10] of chordal graphs. In it, a *contraction* of G is any graph that results from G

by repeating the following operation: *contract* edge xy by deleting xy and replacing the vertices x and y with a new vertex v_{xy} whose neighborhood is $(N_G(x) \cup N_G(y)) - \{x, y\}$ (without creating loops or parallel edges).

Theorem 1.1 ([1, 5, 12]). *A graph G has a clique tree if and only if the 4-cycle C_4 is not a contraction of an induced subgraph of G; in other words, if and only if G is chordal.*

References [2, 10] present the relationship between chordal graphs and their clique trees in detail.

2. Clique series-parallel graphs and clique 2-trees

A graph is *series-parallel* if it contains no subgraph that is isomorphic to a subdivision of K_4 (where a *subdivision* of a graph G is a graph G° that contracts to G where each contracted edge contains a degree-2 vertex of G°—thus, edges of G correspond to internally disjoint paths of G° whose internal vertices are degree-2 vertices). Series-parallel graphs are not required to be 2-connected as well (although this is often done—see [8]); also, all graphs are assumed to be simple—multiple edges and loops are not allowed.

A graph is a 2-*tree* if it can be recursively built up from a single edge by repeatedly creating a new degree-2 vertex that is adjacent to two pre-existing adjacent vertices; for convenience, also consider a graph that consists of a single vertex to be a 2-tree. A *partial* 2-*tree* is a subgraph of a 2-tree. See [2] for other characterizations of these concepts, including the following.

Lemma 2.1 ([7, 13]). *A graph is series-parallel if and only if it is a partial 2-tree* (*and there is a linear algorithm for inserting edges into a series-parallel graph to make it into a 2-tree*).

Define a *clique* 2-*tree* [or *clique partial* 2-*tree*] for a graph G to be a [partial] 2-tree H that has the maxcliques of G as its nodes such that, for every $v \in V(G)$, the subgraph H_v is connected; a clique partial 2-tree can also be called a *clique series-parallel graph*. If G has a clique series-parallel graph, then G will have a clique series-parallel graph that is a subgraph of $K(G)$, but G having a clique 2-tree does not imply that G will have a clique 2-tree that is a subgraph of $K(G)$ (since edges QQ' with $Q \cap Q' = \emptyset$ are allowed in clique 2-trees for G but not in the clique graph $K(G)$). Every clique tree is automatically a clique series-parallel graph, and every clique series-parallel graph is automatically a clique 2-tree.

Figure 1 shows an example of a graph G with a clique series-parallel graph H^- and a clique 2-tree H^+ that contains H^- as a subgraph. (The node label 125 abbreviates the maxclique $\{1, 2, 5\}$ of G and so on.)

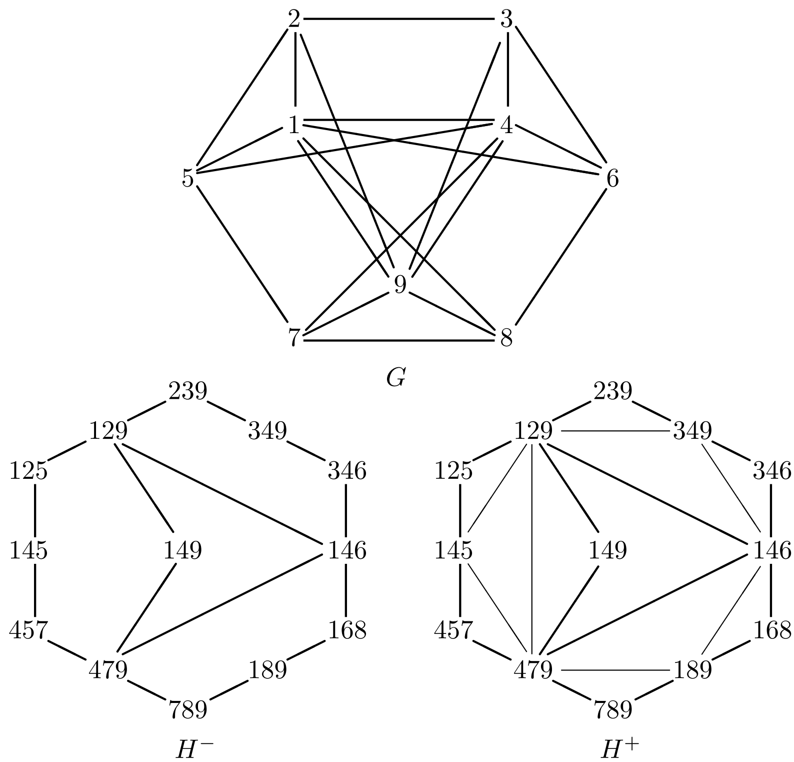

Figure 1: A graph G with a clique series-parallel graph H^- and a clique 2-tree H^+.

Figure 2 shows an example of a graph G that has no clique series-parallel graph (and so no clique 2-tree): If H were a clique series-parallel graph for G, then H would have to contain at least two of the three edges from each of the two triangles in $K(G)$ in order to make H_3 and H_5 connected, and H would have to contain the six edges of $K(G)$ that are not in triangles in order to make the other six H_v subgraphs connected. But none of those possible edge choices would produce a series-parallel graph—there would always be a subgraph isomorphic to a subdivision of K_4.

Lemma 2.2. *A graph has a clique* 2*-tree if and only if it has a clique series-parallel graph.*

Proof. Every clique 2-tree is, of course, a clique series-parallel graph. Conversely, using that an edge QQ' of a clique (partial) 2-tree H is allowed to have $Q \cap Q' = \emptyset$, edges can always be inserted to make a clique series-parallel graph into a clique 2-tree. □

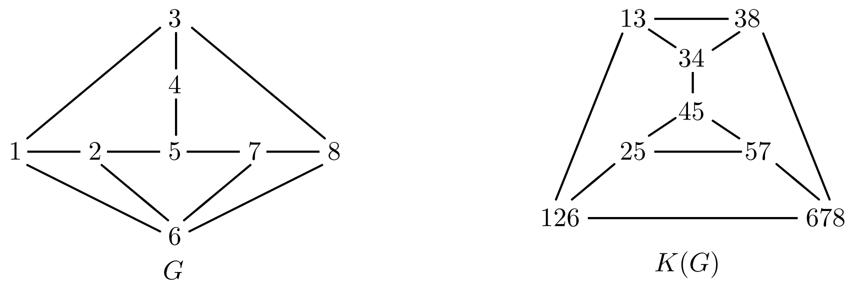

Figure 2: A graph G that has no clique series-parallel graph.

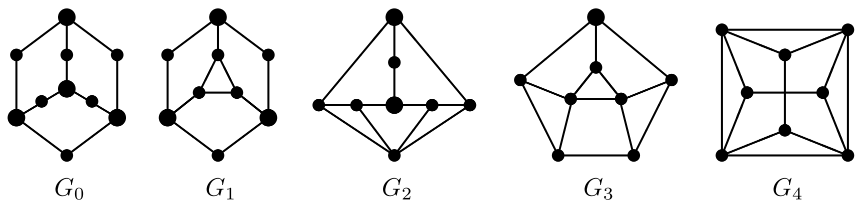

Figure 3: Five graphs that do not have clique 2-trees.

A *claw* is an induced subgraph that is isomorphic to $K_{1,3}$ and the degree-3 vertex of the $K_{1,3}$ the *center* of the claw. Theorem 2.1 will be the clique 2-tree analog of Theorem 1.1, with the graphs shown in Figure 3 replacing C_4. Observe that each graph G_t in Figure 3 has t edge-disjoint triangles and $4-t$ edge-disjoint claws (whose centers are shown as larger vertices) and that G_2 is the graph G in Figure 2.

Theorem 2.1. *A graph G has a clique 2-tree if and only if no graph in Figure 3 is a contraction of an induced subgraph of G.*

Proof. First, suppose that some graph G_t in Figure 3 is a contraction of an induced subgraph of G. Using Lemma 2.2, imagine trying to find a clique series-parallel graph H for G in $K(G)$ [arguing by contradiction].

The t triangles in G_t should correspond to nodes $Q_1, \ldots, Q_t$ of H. [Figure 2 illustrates this for G_2, where the two triangles of G correspond to the nodes $Q_1 = 126$ and $Q_2 = 678$ in $K(G)$.] Say the $4-t$ claws in G_t are $G_{t,1}$, …, $G_{t,4-t}$ and have centers $v_1, \ldots, v_{4-t}$ respectively. The three edges of each $G_{t,i}$ correspond to a triangle Δ_i in $K(G_t)$. [In Figure 2, the claws $G_{2,1}$ and $G_{2,2}$ of G that have centers $v_1 = 3$ and $v_2 = 5$, respectively, correspond to the triangles Δ_1 with nodes $13, 34, 38$ and Δ_2 with nodes $25, 45, 57$.] In order to make each H_{v_i} connected, H would have to contain at least two edges of each Δ_i; let Q'_i be a node that is on two such edges. [For the claw $G_{2,1}$ in Figure 2, H would contain at least two edges from Δ_1, so H would include at least two of the edges 13–34, 13–38, 34–38 and Q'_1 would be one of the nodes 13, 34, 38.]

Thus, H would contain the $t+(4-t)=4$ nodes $Q_1,\ldots,Q_t,Q'_1,\ldots,Q'_{4-t}$ where those four nodes are pairwise connected by a total of six paths in H such that no internal node of one path is a node of another path. Thus, H would contain a subgraph isomorphic to a subdivision of K_4 [contradicting H being series-parallel]. Therefore, G could not have a clique 2-tree.

Conversely, suppose a graph G has no clique 2-tree. Further suppose that G is both vertex deletion minimal and contraction minimal—so deleting any vertex from G or contracting any edge of G would produce a graph that has a clique 2-tree. Therefore, G must be 2-connected (if each block of G had a clique 2-tree, then G would have a clique series-parallel graph and so would have a clique 2-tree by Lemma 2.2).

Because $K(G)$ is not series-parallel (by Lemmas 2.1 and 2.2, since G has no clique 2-tree), $K(G)$ contains a subgraph H that has degree-3 nodes Q_1, Q_2, Q_3, Q_4—each a maxclique of G—such that H is isomorphic to a subdivision of K_4 (and so all nodes of H other than Q_1, Q_2, Q_3, Q_4 have degree 2 in H). The vertex deletion minimality of G implies that each node Q of H contains only enough vertices to make Q have nonempty intersections with two or three other nodes of H. Specifically, the four nodes Q_i have $|Q_i| \in \{2,3\}$, and the other nodes Q of H have $|Q|=2$. Therefore, each node of H *either* has degree 3 and induces a triangle or edge of G *or* has degree 2 and induces an edge of G.

If a degree-3 node Q_i of H induces a triangle of G, then each vertex of that triangle will be adjacent to one vertex outside the triangle (from a node of one of the three paths of H that have Q_i as an endpoint). Now suppose instead that a degree-3 node Q_i of H induces an edge v_iw_i of G, and suppose the maxcliques R'_i, R''_i, R'''_i of G are the neighbors of Q_i in the three paths of H that have Q_i as an endpoint. Without loss of generality, say $v_i \in R'_i \cap R''_i$.Thus, $v_i \notin R'''_i$ and $w_i \in R'''_i$ (otherwise w_i could have been deleted from G, with H modified by deleting the node Q_i and inserting two edges to join one of R'_i, R''_i, R'''_i to the other two so as to make one of them a degree-3 node of H) and $w_i \notin (R'_i \cup R''_i)$ (otherwise $Q_i \subseteq R'_i$ or $Q_i \subseteq R''_i$, contradicting that Q_i, R'_i, R''_i are maxcliques of G). Therefore, v_i is adjacent to vertices $r'_i \in R'_i - R''_i$ and $r''_i \in R''_i - R'_i$ where r'_i and r''_i are nonadjacent (since R'_i and R''_i are maxcliques of G). Moreover, w_i and r'_i are nonadjacent (since r'_i is adjacent to v_i and $\{v_i, w_i\}$ is a maxclique of G). Similarly, w_i and r''_i are nonadjacent, and so $\{v_i, w_i, r'_i, r''_i\}$ induces a claw in G with center v_i.

Also, each of w_i, r_i', r_i'' will be adjacent to one vertex outside the claw (from a node of one of the three paths of H that have Q_i as an endpoint).

Therefore, the four degree-3 nodes Q_1, Q_2, Q_3, Q_4 of H will induce four edge-disjoint subgraphs of G such that, for some $t \in \{0, 1, 2, 3, 4\}$, each maxclique Q_i is one of t triangles or $4 - t$ claws. By the vertex deletion minimality and contraction minimality of G, the vertices of G outside of those four subgraphs will form a total of six paths—each of length 0 or 1—that pairwise connect those four subgraphs. Considering each of the five possible values for t in turn, G must be the graph G_t shown in Figure 3. (Contracting any additional edges of any G_t would produce a graph that has a clique series-parallel graph.) □

3. Clique outerplanar and clique mop graphs

A graph is *outerplanar* if it has a plane embedding with all vertices on one face. Thus, a 2-connected graph is outerplanar if and only if it has a hamiltonian cycle C such that every edge of the graph either is an edge of C or is a chord of C that has no crossing chord. By [3], a graph is outerplanar if and only if it contains no subgraph that is isomorphic to a subdivision of K_4 or $K_{2,3}$. Thus, every outerplanar graph is series-parallel (and $K_{2,3}$ is a series-parallel graph that is not outerplanar).

A graph is a *maximal outerplanar graph*—often abbreviated as a *mop graph*—if it is outerplanar but inserting an additional edge would always create a graph that is not outerplanar. Equivalently, a graph is a mop graph if and only if it is a 2-tree with no edge in three triangles. Notice that outerplanar graphs can also be called *partial mop graphs* and that every [partial] mop graph is a [partial] 2-tree.

Define a *clique mop graph* [or *clique partial mop graph*] for a graph G to be a [partial] mop graph H that has the the maxcliques of G as its nodes such that, for every $v \in V(G)$, the subgraph H_v is connected; a clique partial mop graph can also be called a *clique outerplanar graph*. If G has a clique outerplanar graph, then it will have a clique outerplanar graph that is a subgraph of $K(G)$, but G having a clique mop graph does not imply that G will have a clique mop graph that is a subgraph of $K(G)$ (since edges QQ' with $Q \cap Q' = \emptyset$ are allowed in clique mop graphs for G but not in the clique graph $K(G)$). Every clique tree is automatically a clique outerplanar graph, every clique outerplanar graph is automatically a clique series-parallel graph, and every clique mop graph is automatically a clique 2-tree.

The graphs H^- and H^+ in Figure 1 are not clique (partial) mop graphs—neither is even outerplanar. Figure 4 shows an example of a graph G that

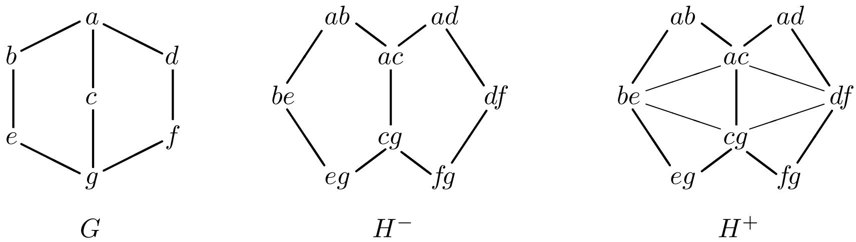

Figure 4: A graph G with a clique outerplanar graph H^- and a clique mop graph H^+.

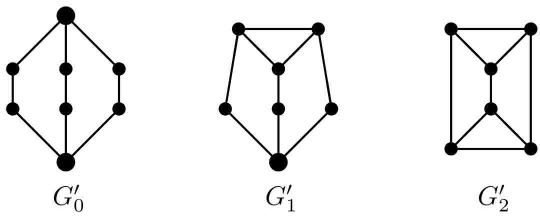

Figure 5: Three graphs that have clique 2-trees but not clique mop graphs.

has a clique outerplanar graph H^- and a clique mop graph H^+ that contains H^- as a subgraph.

Lemma 3.1. *A graph has a clique mop graph if and only if it has a clique outerplanar graph.*

Proof. Every clique mop graph is, of course, a clique outerplanar graph. Conversely, edges can be inserted into any outerplanar graph so as to make it into a mop graph (see [6] for an algorithmic discussion) and so edges can always be inserted to make a clique outerplanar graph into a clique mop graph. □

Theorem 3.1 will be the clique 2-tree analog of Theorem 1.1, with the graphs shown in Figures 3 and 5 replacing C_4. Observe that each graph G'_t in Figure 5 has t vertex-disjoint triangles and $2 - t$ vertex-disjoint claws (whose centers are shown as larger vertices).

Theorem 3.1. *A graph G has a clique mop graph if and only if no graph in Figure 3 or Figure 5 is a contraction of an induced subgraph of G.*

Proof. First, suppose that some graph G_t in Figure 3 or G'_t in Figure 5 is a contraction of an induced subgraph of G. In the G_t case, Theorem 2.1

shows that G would have no clique 2-tree and so no clique mop graph. Thus, assume G'_t is a contraction of an induced subgraph of G, and using Lemma 3.1, imagine trying to find a clique outerplanar graph H for G in $K(G)$. The argument proceeds as in the proof Theorem 2.1, except now with t triangles and $2-t$ claws where H would contain $t+(2-t)=2$ degree-3 nodes connected by three paths in H, and so H would contain a subgraph isomorphic to a subdivision of $K_{2,3}$ (contradicting H being outerplanar). Therefore, G could not have a clique mop graph.

Conversely, suppose a graph G has no clique mop graph but using Theorem 2.1, has a clique 2-tree (toward showing that one of the three graphs in Figure 5 is a contraction of an induced subgraph of G). Further suppose G is both vertex deletion minimal and contraction minimal. The argument proceeds as in the proof of Theorem 2.1, except H is now isomorphic to a subdivision of $K_{2,3}$ with two degree-3 nodes Q_1 and Q_2 where, for some $t \in \{0,1,2\}$, each maxclique Q_i is one of t triangles or $2-t$ claws. By the vertex deletion minimality and contraction minimality of G, the vertices of G outside of those two subgraphs will form three paths—each of length 0 or 1—that connect those two subgraphs. Considering each of the three possible values for t in turn, G must be the graph G'_t shown in Figure 5. (Contracting any additional edges of any G'_t would produce a graph that has a clique outerplanar graph.) □

4. Practicality and applicability

The greedy minimum spanning tree construction of the clique trees of chordal graphs (see [10, §2.1]) underlies the traditional applications of chordal graphs as surveyed in [10, §2.4]. (Edges are chosen by Kruskal's algorithm—heaviest-weight-first, avoiding forming cycles—where the weight of the edge QQ' is $|Q \cap Q'|$.) But a similar greedy construction fails for clique series-parallel graphs and clique outerplanar graphs. (If a clique series-parallel graph H is constructed for the graph G in Figure 1 by first choosing the edges that are shown there in H^-, except with the weight-1 edge 129–189 chosen instead of the weight-1 edges 129–146 and 146–479, then those fifteen edges make each H_v with $v \neq 4$ connected, but no further edges can be chosen so as to make H_4 connected as well while preserving H being series-parallel.)

Even finding all the maxcliques of a nonchordal graph can present computational problems: The generalized octahedron $K_{2,\ldots,2}$ of order $2n$—which does have a clique series-parallel graph by Lemma 2.2 and Theorem 2.1—has 2^n maxcliques. (By way of contrast, every chordal graph of order n has at most n maxcliques, and they can be found in linear time.)

On the positive side, a fairly recent application of clique trees in systems biology (see the detailed account in [14], the more general survey in [11], or the brief description in [9]) can potentially use clique series-parallel graphs instead of clique trees. In the existing form of this application, a protein interaction graph G leads to a clique tree H whose nodes represent "functional groups" of proteins that correspond to "snapshots of protein associations" during some sort of a dynamic process. (If G does not have a clique tree, then edges are inserted in order to make G chordal.) The clique tree H "elucidat[es] temporal relations between functional groups", ... "tracking a protein's path through a cascade of functional groups" [14]. Yet this application does not make a particular case for requiring H to be a tree (indeed, there a reluctance "to impose an artificial order between functional groups", as would occur in a clique tree).

Modifying this application to allow H to be a series-parallel graph could be useful in light of a characterization from [4]:

> A 2-connected graph H is series-parallel if and only if the arbitrary orientation of any edge e of H determines a unique orientation of $E(H)$ such that the set of directed cycles is exactly the set of cycles that contain e (in other words, a unique orientation with no other edge e' such that e and e' are directed consistently in one cycle yet are directed oppositely in another cycle).

In the biological application, this means that knowing or positing the temporal relation—the direction in which proteins move—between two arbitrary functional groups that are adjacent in a 2-connected clique series-parallel graph for a protein interaction graph will imply the temporal relations among all adjacent functional groups.

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