

## THE ENUMERATION OF MAXIMAL CLIQUES OF LARGE GRAPHS\*

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**Abstract.** An algorithm for enumerating maximal cliques (complete subgraphs) is proposed. The aim is to deal with the difficulties caused by the size of the problem.

**Key words.** Algorithms, clique, enumeration, graph.

**1. Introduction.** The problem considered here is best formulated in terms of an undirected graph  $G$  (Fig. 1). If  $S_0$  is the set of nodes and  $E$  the set of edges, the goal is to identify completely connected subgraphs (or cliques) which are maximal.

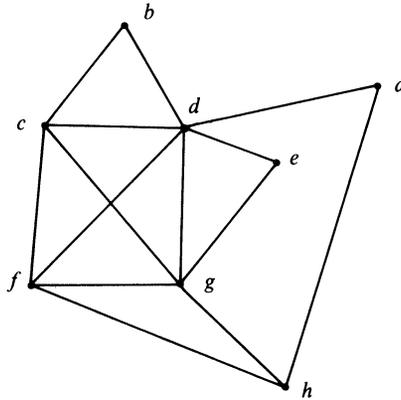


FIG. 1

More generally,  $S_0$  is a set of elements, and there is defined over pairs in  $S_0$  a symmetric, nontransitive binary relation  $R$ . ( $E$  is a set of pairs which are in relation  $R$ .) A subset  $S$  of  $S_0$  is a *maximal subset* (ms) if

- (i) every pair in  $S$  is in relation  $R$ , and
- (ii)  $S$  is not a proper subset of any set with property (i).

The ms are of interest in many contexts: graph theory (the coloring problem), switching theory (state minimization [1]), operations research (scheduling [2], [3]), information systems, etc. There are several known algorithms [1], [4], [5], [6] for enumerating these sets. As a rule, however, these algorithms cannot handle large problems [3] efficiently. The difficulty arises because the terms generated include duplications, or even submaximal sets. To avoid this, a list of all the terms has to be kept and repeatedly scanned. In the worst cases, the list cannot be accommodated in core.

This paper proposes a new algorithm which is especially efficient in dealing with large problems, and has none of the shortcomings mentioned above. The set generated corresponds precisely (and without duplications) to the set desired.

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To verify: if both statements were true, the ms would include one of the disallowed pairs,  $ac$ ,  $ce$ ,  $ch$ . If neither were true, the addition of  $c$  to this term could not possibly violate a constraint, so that the term could not have been maximal.

Consider next row  $b$ . An ms which includes  $b$  cannot include any of  $a$ ,  $e$ , or  $h$  since  $\{a, e, h\} \subset D_b$ . This, together with the above, means that every ms which includes  $b$  must also include  $c$ . To generalize, we state:

*If  $D_x \subseteq D_y$ , then  $x$  occurs in every ms where  $y$  occurs.*

Further notation is introduced at this point in order to facilitate the manipulation of subsets of  $\mathcal{M}$  according to certain characteristics. For  $S \subseteq S_0$ , let  $L(S)$  denote "the set of all ms which include *at least one* element of  $S$ ." Similarly, let  $E(S)$  denote "the set of all ms which include *every* element of  $S$ ." Thus,

$$L(S) = \{M | M \in \mathcal{M}, S \cap M \neq \emptyset\},$$

$$E(S) = \{M | M \in \mathcal{M}, S \subseteq M\}.$$

The following relations are direct consequences of these definitions:

- (1)  $L(\{x\}) = E(\{x\})$ ,
- (2)  $E(S_1) \cap E(S_2) = E(S_1 \cup S_2)$ ,
- (3)  $L(S_1) \cap L(S_2) = L(S_1)$  if  $S_1 \subseteq S_2$ ,
- (4)  $L(\emptyset) = \emptyset$ .

Also, since any ms which includes  $x$  can only include elements in  $C_x$ , we can write

$$E(\{x\}) \cap L(S) = \begin{cases} E(\{x\}) & \text{if } x \in S, \\ E(\{x\}) \cap L(S \cap C_x) & \text{otherwise.} \end{cases}$$

More generally,

$$(5) \quad E(\{x\}) \cap \left( \bigcap_i L(S_i) \right) = E(\{x\}) \cap \left( \bigcap_{i: x \notin S_i} L(S_i \cap C_x) \right).$$

**3. Enumeration through disjoint subproblems.** In the previous example, where  $S_0 = \{a, b, c, d, e, f, g, h\}$ , the set of all ms can be written

$$\mathcal{M} = L(S_0) = L(\{a, b, c, d, e, f, g, h\}),$$

which simply states that  $\mathcal{M}$  is the set of all ms which include at least one element. As discussed above,  $\mathcal{M}$  has two disjoint subsets,

- (i) all ms which include  $\{c\}$ ,
- (ii) all ms which include at least one of  $\{a, e, h\}$ ,

and this is expressed by writing,

$$\mathcal{M} = L(S_0) = E(\{c\}) \cup L(\{a, e, h\}).$$

To formalize this notion, we write

$$(6) \quad L(S \cup \{x\}) = E(\{x\}) \cup (L(S) \cap L(D_x)).$$

Here, the right-hand side is the union of disjoint sets: all ms which include  $x$ , and all which exclude  $x$  but include some element in  $S$ .

In what follows, the notation will be simplified by writing  $L(a, b, \dots, x)$  instead of the formally correct  $L(\{a, b, \dots, x\})$ , etc. Equations (1) through (6) can be used to reduce the problem of enumerating  $\mathcal{M}$  into a series of smaller problems. The key step is the substitution specified by (6) which is applied repeatedly. For the problem in Fig. 3, we have

$$\begin{aligned}\mathcal{M} &= L(a, b, c, d, e, f, g, h) = E(c) \cup L(a, e, h) \\ &= E(c) \cup E(a) \cup (L(e, h) \cap L(b, c, e, f, g)) \\ &= E(c) \cup E(a) \cup ((E(e) \cup L(h) \cap L(a, b, c, f, h)) \cap L(b, c, e, f, g)).\end{aligned}$$

Since  $L(h) = E(h)$ , equation (5) allows the reductions

$$\begin{aligned}E(e) \cap L(b, c, e, f, g) &= E(e), \\ E(h) \cap L(a, b, c, f, h) \cap L(b, c, e, f, g) &= E(h) \cap L(f, g), \\ \mathcal{M} &= E(c) \cup E(a) \cup E(e) \cup (E(h) \cap L(f, g)).\end{aligned}$$

Now  $L(f, g) = E(f) \cup (L(g) \cap L(a, b, e))$ , so that we write,

$$\begin{aligned}E(h) \cap L(f, g) &= (E(h) \cap E(f)) \cup (E(h) \cap L(g) \cap L(a, b, e)), \\ \mathcal{M} &= E(c) \cup E(a) \cup E(e) \cup (E(h, f) \cup (E(h) \cap L(g) \cap L(a, b, e))).\end{aligned}$$

Using equation (5), we have

$$E(h) \cap L(g) \cap L(a, b, e) = E(h) \cap L(g) \cap L(a).$$

Finally, since  $L(g) \cap L(a) = E(g) \cap L(a) = \emptyset$ , we obtain

$$\mathcal{M} = E(c) \cup E(a) \cup E(e) \cup E(h, f).$$

The problem is thus reduced to four smaller problems whose solutions correspond to disjoint subsets of  $\mathcal{M}$ . Each of these can now be solved separately and the complete solution  $\mathcal{M}$  obtained.

In evaluating  $E(a)$ , for example, only the set  $C_a$  need be considered. This corresponds to Fig. 4 whose ms set is  $\{d, h\}$ . The addition of  $a$  to every member of this set yields  $E(a) = \{ad, ah\}$ . Similarly,  $E(h, f)$  is obtained by adding  $h$  and  $f$  to each term of the ms set derived from Fig. 5 which consists of variables in  $C_h \cap C_f$  alone. This ms set is simply  $\{g\}$  so that  $E(h, f) = \{fgh\}$ .

To generalize, let  $S$  be a set for which  $x, y \in S$  implies  $x \in C_y$ . Then,

$$(7) \quad E(S) = \begin{cases} S & \text{if } \bigcap_{x \in S} C_x = \emptyset, \\ E(S) \cap L(\bigcap_{x \in S} C_x) & \text{otherwise.} \end{cases}$$

**4. Enumeration algorithm.** This section formalizes the approach outlined above by giving an algorithm for enumerating  $\mathcal{M}$ . The algorithm manipulates

$D_x$	$x$	$C_x$
$h$	$d$	—
$d$	$h$	—

FIG. 4

$D_x$	$x$	$C_x$
—	$g$	—

FIG. 5

symbolic expressions composed of  $E$ - and  $L$ -sets. The data base consists of the sets  $S_0$ ,  $C_x$  and  $D_x$ , for  $x \in S_0$ . The algorithm is organized around a pushdown stack which serves to store partially formulated disjoint subproblems. Items on the stack are expressions involving sets of the form  $E(S)$  and  $L(S)$ . A possible item on the stack could be

$$E(h) \cap L(g) \cap L(a, b, e).$$

Specifically, each item on the stack is a multiple set intersection between one or more  $L$ -sets and at most one  $E$ -set.

Starting with the expression  $L(S_0)$ , the algorithm consists of repeated applications of equations (6) and (7), supplemented by the reduction equations (1) through (5). Equation (6) is used to split an expression into two others which correspond to disjoint subsets of the original set; these are then pushed on the stack, and the process is repeated until an expression of the form  $E(S)$  is obtained. Equation (7) is then applied once.

**ALGORITHM A.**

Input:  $S_0, \{C_x | x \in S_0\}, \{D_x | x \in S_0\}$ .

Output:  $\mathcal{M}$ .

Step 1 (Initialize). Place  $L(S_0)$  on the stack.

Step 2 (Prepare to split). (a) If the stack is empty, stop.

(b) Unload the top expression from the stack and call it  $T$ .  $T$  is a multiple intersection whose form is either

$$E(S') \cap \left( \bigcap_{i \in I} L(S_i) \right)$$

or simply

$$\bigcap_{i \in I} L(S_i).$$

In the first case set  $V = S'$ , in the second case set  $V = \emptyset$ .

Step 3 (Choose the  $L$ -term to be split). (a) Select  $k \in I$  so that  $S_k$  has the fewest elements possible. Also choose  $x \in S_k$ , and let  $S = S_k - \{x\}$ .

(b) If  $S = \emptyset$  go to Step 5. (Equation (1) can be applied instead of equation (6).)

Step 4 (Formulate the second subproblem). (a) Compute

$$Q = \begin{cases} D_x & \text{if } V = \emptyset, \\ D_x \cap (\bigcap_{y \in V} C_y) & \text{otherwise.} \end{cases}$$

(b) If  $Q = \emptyset$  go to Step 5. (Every  $m_s$  which covers  $V$  also covers  $\{x\}$ .)

(c) Make a copy of  $T$  with  $L(S) \cap L(Q)$  substituted for  $L(S_k)$ , and load this copy on the stack.

*Step 5* (Formulate the first subproblem). (a) Let  $J = \{j | j \in I, x \in S_j\}$ . If  $J = \emptyset$  go to *Step 6*. (Equation (7) is applicable.)

(b) For all  $j \in J$  compute  $W_j = S_j \cap C_x$ . If  $W_j = \emptyset$  for any  $j \in J$  go to *Step 2*. (No ms covers both  $V$  and  $\{x\}$ .)

(c) Place the expression

$$E(V \cup \{x\}) \cap \left( \bigcap_{j \in J} L(W_j) \right)$$

on the stack and go to *Step 2*.

*Step 6* (Apply equation (7).) (a) Compute

$$P = \bigcap_{y \in V \cup \{x\}} C_y.$$

(b) If  $P = \emptyset$  output  $V \cup \{x\}$ , then go to *Step 2*.

(c) Load the stack with  $E(V \cup \{x\}) \cap L(P)$ , and go to *Step 2*. (End Algorithm A.)

In practice, rather than compute the set

$$\bigcap_{y \in V} C_y$$

each time, it is more convenient to store it along with the associated item on the stack.

**5. Conclusion.** Techniques for generating maximal subgraphs were discussed with reference to the difficulties caused by the size of the problem. An effective procedure was proposed for systematically reducing these problems into smaller ones whose ms sets are disjoint. An important feature of the enumeration algorithm is that it is organized around a stack, so that its core requirements are minimal.

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