Abstract

A clique in a graph is a set of vertices, each of which is adjacent to every other vertex in the set. A $k$-clique relaxes this requirement, requiring vertices to be within a distance $k$ of each other, rather than directly adjacent. In theory, a maximum clique algorithm can easily be adapted to solve the maximum $k$-clique problem. We use a state of the art maximum clique algorithm to show that this is feasible in practice, and introduce a lazy global domination rule which sometimes vastly reduces the search space. We include experimental results for a range of real-world and benchmark graphs, and a detailed look at random graphs.

1 Introduction

A clique in a graph is a set of vertices, each of which is adjacent to every other vertex in the set. Finding a clique of maximum size in a graph is one of the basic NP-hard problems \cite{garey_johnson_1990}; applications include geometry, coding theory, computer vision and bioinformatics \cite{bryan_baker_perrig_patterson_1999,bryan_waltz_2006}. However, when analysing real-world data, a clique may be too strong a requirement. A $k$-clique (or sometimes $n$-clique or $s$-clique) is a relaxed form of clique, where instead of requiring each pair of vertices to be directly adjacent, we only require that they be connected by a path of length at most $k$ \cite{Lucas_1950}. Thus a 1-clique is a clique, a 2-clique may be thought of as “a group of people, all of whom either know each other or have a mutual acquaintance”, and so on. We illustrate this in Figure 1. Determining the size of a maximum $k$-clique is NP-hard for any fixed $k$ \cite{bryan_lamprou_palma_2002}.

A related relaxation is a $k$-club, which tightens the requirement of a $k$-clique as follows \cite{mok_kocay_1979}. In a $k$-clique, each pair of vertices is connected by a path of length at most $k$, but that path may use any vertices in the original graph. In a $k$-club, each pair of vertices must be connected by a path of length at most $k$ using only vertices that are also in the club. Thus the 2-clique in Figure 1 is not a 2-club (obviously, every $k$-clique is a $k$-clique).

A recent survey by Shahinpoor and Butenko discusses algorithms and results for $k$-clique and $k$-club problems \cite{shahinpoor_butenko_2013}. We adopt their notation of $\tilde{\omega}_k$ for the size of a maximum $k$-clique; the use of $\omega$ for the size of a maximum clique is standard. They note that “unlike the maximum clique problem, the maximum $s$-clique problem has not been the subject of extensive research and we are not aware of any computational

Figure 1: On the left, a graph, with its unique maximum clique $\{1,2,5,8\}$ of size 4 highlighted. On the right, the same graph, with a maximum 2-clique $\{1,2,3,4,5,6,8\}$ of size 7 highlighted. This is not a 2-club, since the only path of length 2 between vertices 3 and 6 goes through vertex 7. A 3-clique covers the entire graph.

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results for this problem to date”. This is in contrast to the $k$-club problem, for which a wide range of computational results are available [BLP06, BLP02, MB12, HKN12, CHLS13, SB13, Wot14].

A maximum clique algorithm can easily be adapted to find a maximum $k$-clique in a graph $G$ by considering the graph $G^k$, which we describe below. However, it is not obvious that this is a viable approach: even if $G$ is sparse, $G^k$ may not be, and the maximum clique problem on dense graphs can be very challenging computationally. Here we take a state-of-the-art maximum clique algorithm which is suitable for use on dense graphs [Pro12, MP13], and investigate whether this approach is feasible in practice. We modify the algorithm to include a new lazy “global domination” inference step—this technique provides no benefit for typical maximum clique problems, but for maximum $k$-clique graphs it sometimes gives improvements of several orders of magnitude. We present computational results for the maximum $k$-clique problem on a range of benchmark and real-world graphs. We finish with a detailed look at random graphs.

Throughout, our graphs are finite, undirected, and contain no loops. If $G$ is a graph with vertex set $V$ and edge set $E$, we may write $V(G)$ to mean $V$. The *neighbourhood* of a vertex $v$ in a graph $G$, written $N_G(v)$, is the set of vertices adjacent to $v$. The *degree* of a vertex is the cardinality of its neighbourhood. The density of a graph, denoted $D$, is the proportion of distinct pairs of vertices which have an edge between them. The subgraph *induced by* a set of vertices $W$ is the subgraph with vertex set $W$, and all edges from the original graph that are between pairs of vertices in $W$. If $A$ and $B$ are sets of vertices, we write $A \setminus B$ for the set of vertices which are in $A$ but not $B$, and we write $A + v$ and $A − v$ for $A \cup \{v\}$ and $A \setminus \{v\}$ respectively.

2 Algorithms

Our approach for finding a maximum $k$-clique is presented as Algorithm 1. Our first step (line 3) is to replace our input graph $G$ with a modified graph $G^k$. This graph has the same vertex set as $G$, and edges between any two distinct vertices $v_1$ and $v_2$ if there is a path of length at most $k$ between $v_1$ and $v_2$ in $G$. We may construct this graph using a bounded breadth-first search: we refer to Chang et al. [CHLS13] for how to implement this quickly in practice. Now it is easy to see that maximum cliques in $G^k$ correspond with maximum $k$-cliques in $G$ [BBT05].

**Colouring** The current state-of-the-art for the maximum clique problem on dense graphs, due to Tomita et al. [TS03, TK07, TSH+10], is to use branch and bound with a greedy graph colouring. A *colouring* of a graph is an assignment of colours to vertices, such that adjacent vertices are given different colours; if we can colour a graph using $c$ colours, then the graph cannot contain a clique of size greater than $c$ (each vertex in a clique must be given a different colour).

Obtaining a minimal colouring is *NP*-hard, but we may create a greedy colouring in polynomial time. This is done by the *colourOrder* routine: we start the first colour (line 29), and while there are uncoloured vertices remaining (line 30), we try to give each vertex in turn the current colour (lines 31 to 36). When we cannot colour any further vertices, we start a new colour (line 37).

The key step in Tomita’s algorithms is to produce a constructive colouring, which is used in a clever way. The *colourOrder* routine does not just return the number of colours used. Instead, it returns a pair of arrays, *order* and *bounds*. The *order* array contains vertices, in the order in which they were coloured. The $i$th entry of the *bounds* array contains the colour number used for the $i$th vertex in *order*. We illustrate this in Figure 2. Crucially, *bounds* is non-decreasing (i.e. $\text{bounds}[i+1] \geq \text{bounds}[i]$), and we may colour the subgraph induced by the first $i$ vertices of *order* using *bounds*[i] colours.

The order in which vertices are selected for colouring can have a large effect upon performance. Various initial vertex orderings have been considered for the maximum clique problem—we refer to a computational study by Prosser for details [Pro12]. Here we will colour vertices in a static non-increasing degree order, which we do by permuting the graph at the top of search (line 4). We will not be using Tomita et al.’s dynamic tie-breaking mechanism [TSH+10]: although doing so can sometimes be beneficial for small dense graphs in a maximum clique context, for the larger graphs we will be considering here the cubic cost is prohibitively expensive. For the same reason, we use a simple greedy colouring and do not use Tomita et al.’s (cubic) colour repair step [TSH+10].

**Branching and recursing** We may now describe the main recursive part of the algorithm. If $v$ is a vertex, then a clique in $G^k$ either contains only $v$ and vertices adjacent to $v$, or does not contain $v$. This allows us to grow cliques by repeatedly picking a vertex, and branching upon whether or not to include
Algorithm 1: An algorithm for the maximum $k$-clique problem.

maximumKClique :: (Graph $G$, Integer $k$) $\rightarrow$ Vertex Set

begin

$G \leftarrow G^k$

permute $G$ so that vertices are in non-increasing degree order

global $C^* \leftarrow \emptyset$

expand($\emptyset, V(G)$)

return $C^*$ (unpermuted)

end

expand :: (Vertex Set $C$, Vertex Set $P$)

begin

$(order, bounds) \leftarrow \text{colourOrder}(P)$

$v_{\text{rej}} \leftarrow \text{unset}$

for $i \leftarrow |P|$ downto 1 do

if $|C| + bounds[i] \leq |C^*|$ then return

if $v_{\text{rej}} \neq \text{unset}$ then

$P \leftarrow P \setminus \{w \in V(G) : N_G(w) - v_{\text{rej}} \subseteq N_G(v_{\text{rej}}) - w\}$

$v \leftarrow order[i]$

if $v \in P$ then

$C \leftarrow C + v$

if $|C| > |C^*|$ then $C^* \leftarrow C$

$P' \leftarrow P \cap N_G(v)$

if $P' \neq \emptyset$ then expand($C, P'$)

$C \leftarrow C - v$

$P \leftarrow P - v$

$v_{\text{rej}} \leftarrow v$

end

end

colourOrder :: (Vertex Set $P$) $\rightarrow$ (Vertex Array, Int Array)

begin

$(order, bounds) \leftarrow ([], [])$

$\text{uncoloured} \leftarrow P$

$\text{colour} \leftarrow 1$

while $\text{uncoloured} \neq \emptyset$ do

$\text{colourable} \leftarrow \text{uncoloured}$

while $\text{colourable} \neq \emptyset$ do

$v \leftarrow$ the first vertex of $\text{colourable}$

append $v$ to $\text{order}$, and append $\text{colour}$ to $\text{bounds}$

$\text{uncoloured} \leftarrow \text{uncoloured} - v$

$\text{colourable} \leftarrow \text{colourable} \cap N_G(v)$

$\text{colour} \leftarrow \text{colour} + 1$

end

end

return $(\text{order}, \text{bounds})$
it. Our growing clique is stored in the variable $C$, which is initially empty (line 5). We also track which vertices may still be added to $C$ in the variable $P$, which initially contains every vertex (line 3). The \textbf{expand} procedure picks a vertex $v$ (line 14), then considers adding $v$ to $C$ (lines 15 to 24): we create a new $P'$ from $P$ (line 20) by rejecting vertices which are not adjacent to $v$ (and thus every vertex in $P'$ is adjacent to every vertex in $C$). If vertices remain in $P'$, we recurse (line 21). We then take the opposite branch choice, and consider rejecting from $P$ and $C$ (lines 22 to 23). We then loop, and pick a new $v$.

**Integrating the colour bound** We keep track of the best solution we have found so far, which we call the \textit{incumbent}; this is stored in $C^*$, which is initially empty (line 5). Whenever we find a new clique, we compare its size to that of $C^*$, and if it is better, the incumbent is unseated (line 10). Now we may make use of the colour bound. At the start of the recursive procedure (line 11), we use \textbf{colourOrder} to produce a constructive greedy colouring of the subgraph induced by $P$ into the array \textit{order}, with the colour numbers placed in \textit{bounds}. When selecting $v$, we iterate over \textit{bounds} from right to left (line 12). Now on line 13 we know that the largest possible clique we could find at the current location has size no greater than $|C| + \textit{bounds}[i]$, so if this cannot unseat the incumbent then we may abandon search and backtrack.

**Lazy global domination** Aside from the $G^k$ step, what we have described so far is a standard maximum clique algorithm, and all we have done is opted out of certain more computationally expensive inference steps (more complicated initial vertex orderings, and cubic colourings). If we ignore the lines shown in blue, we obtain the maximum clique algorithm variation that Prosser [Pro12] calls “MCSa1”.

Now we will introduce a new lazy global domination rule which performs additional inference during search. This rule is not specific to the maximum $k$-clique problem, and is also valid for the maximum clique problem.

Let $v$ and $w$ be distinct vertices in a graph $G$ (they may or may not be adjacent). We say that $v$ \textit{dominates} $w$ if the neighbourhood of $w$, excluding $v$, is a (possibly non-strict) subset of the neighbourhood of $v$, excluding $w$. From a maximum clique perspective, this means that $v$ is “better than” $w$. If $v$ and $w$ are adjacent, any clique containing $w$ may always be extended by the inclusion of $v$; if $v$ and $w$ are non-adjacent, replacing $w$ with $v$ in any clique containing $w$ cannot reduce the amount by which the clique may be grown.

Suppose a graph does contain one or more pairs of dominating vertices. We could make use of this fact during search in at least two ways. Firstly, when accepting a vertex $w$, we may also unconditionally accept any vertex $v$ which dominates $w$. Secondly, when rejecting a vertex $v$, we may also unconditionally reject any vertex $w$ which is dominated by $v$. We could also choose to calculate domination globally (i.e. with respect to $G^k$, or even the original $G$), or locally (i.e. with respect to the subgraph of $G^k$ induced by $C \cup P$).

Detecting whether one vertex dominates another may be done in linear time (we discuss this further below), but finding all vertices dominated by a particular vertex is quadratic, and finding all dominations is cubic. This is a heavy price to pay, if there are no dominating vertices. This is why such a rule has not previously been used in the maximum clique context: in the authors’ experience, most graphs typically considered for the maximum clique problem do not contain dominating vertices, and those that do are too easy computationally for the step to be worthwhile.

However, some of the graphs we consider in the following section \textit{do} contain dominating vertices, so we should consider implementing such a rule. Suppose a dominating pair is found, we iterate over the two indices of the \textit{colourOrder} array which have the greatest value, and if the dominating vertex has a greater index, we reject the dominated vertices. We assume for simplicity that the dominating vertices are always the last two entries of the \textit{colourOrder} array, and that the dominated vertices are the first two entries of the \textit{colourOrder} array. As noted above, this dominates the \textit{colourOrder} array, and so the same domination applies.

**Figure 2:** The graph on the left has been coloured greedily, using four colours: vertices 1, 3, 4 then 6 were given the first colour, then vertices 2 then 7 were given the second colour, then vertex 5 was given the third colour, and vertex 8 the fourth colour. The \textit{order} array contains the vertices in the order they were coloured; the $i$th entry of the \textit{bounds} array contains the number of colours used to colour the first $i$ vertices of \textit{order}. 

| Vertices in colour order | order: | bounds: |
|--------------------------|--------|---------|
| 1 2 3 4 5 6 7 8          | 1 3 4 6 2 7 5 8 |
| Number of colours used   | 1 1 1 2 2 2 3 4 |
and although the maximum clique problem is trivial on these graphs, the maximum \( k \)-clique problem is not for some values of \( k \). Preliminary experiments suggested that the use of a domination rule could be extremely beneficial in certain circumstances, but that in cases where it had little effect, doing such a calculation introduced a substantial penalty to runtimes. Moreover, even in graphs where dominating vertices are present, knowing this fact is sometimes not useful: it is common for an optimal solution to be found straight away, and for the bound to be strong enough to prove optimality immediately, so no branching occurs.

This motivates the design of a lazy global domination rule. We perform our domination checks globally, with respect to \( G^k \) (which may contain more dominating vertices than \( G \)), and we remember and reuse the results of any domination checks we perform. We also only perform inference on the “reject” case, to avoid introducing any cost when a solution is found and proven optimal without branching.

The lines marked in blue in Algorithm 1 show how this is done. When a vertex \( v_{\text{rej}} \) is rejected, we remove from \( P \) any vertex that is dominated (with respect to \( G^k \)) by \( v_{\text{rej}} \). This is line 15—the set of dominated vertices calculated here should be cached. One might expect that this calculation would appear after line 23. However, this introduces a cost if the bound allows the next choice of \( v \) to be eliminated. Thus we simply remember that we have rejected \( v \) by storing it in \( v_{\text{rej}} \) (line 24), and lazily postpone the filtering until after the bound has been checked.

Finally, note that we do not perform a new colouring when we reject dominated vertices—doing so typically does not lead to a smaller bound, since most colour classes contain many vertices. Thus when we select a \( v \) from order, it is now possible that \( v \) has already been rejected. We check for this on line 17.

### Bitset encoding
San Segundo et al. [SSRLJ11, SSMRLH13] observed that the performance of Tomita’s algorithms could be enhanced substantially by using a bitset encoding to obtain a form of SIMD-like parallelism, without altering the steps taken. We have taken such an approach here too, although we do not describe it explicitly—when permuting \( G \) on line 4, the graph should be re-encoded as an array of adjacency bitsets. (It is not helpful to do this before constructing \( G^k \).) Now the intersection on line 20 becomes a simple bitwise “and” operation, and the intersection with complement on line 36 is a bitwise “and not” operation. This is beneficial when testing for dominance, too: each bit in the dominated set on line 15 may be determined by a bitwise “and not”, unsetting a bit, and testing whether the result is empty; the set difference is again a bitwise “and not” operation.

### 3 Experimental Results
Here we give experimental results on a range of standard benchmarks, and on real-world and random graphs. Where timing results are reported, the experiments were run on a machine with Intel E5645 processors, and single-threaded runtimes are given. The time taken to read in the graph from a file is excluded, but preprocessing time (including the construction of \( G^k \) and the bitset encoding) is included. We use the term \textit{nodes} to refer to the number of recursive calls made by the branch-and-bound part of the algorithm.

#### 3.1 Real-World Graphs
We begin with a selection of real-world and standard benchmark graphs. We look at \( k \) equal to 2, 3 and 4 in every case—this is a standard practice for the \( k \)-club problem [CHLS13, Wot14].

**Erdős collaboration graphs** In the first part of Table 1 we present experimental results from Erdős collaboration graphs from the Pajek dataset by Vladimir Batagelj and Andrej Mrvar [1]. We were able to solve all of these problems in under eight minutes (and all but three in under two seconds) when using the domination rule. However, using the unmodified maximum clique algorithm, two of these results did not finish running within one day. Note that for \( k = 4 \), a \( k \)-clique covers all of “Erdos02”.

In several cases, the algorithm found and proved an optimal solution immediately (\( \tilde{\omega} \) is equal to the number of search nodes). This illustrates the necessity of laziness: if we simply computed dominating pairs upfront, we would be paying a cubic preprocessing cost for an algorithm which is effectively quadratic in practice.

[1] http://vlado.fmf.uni-lj.si/pub/networks/data/
Table 1: Experimental results for a range of graphs. For each graph, we consider $k$ equal to 2, 3 and 4. In each case we show the density of $G_k$, and then for both the unmodified algorithm and the algorithm with our lazy global domination step, we give the size of a maximum $k$-clique, the number of nodes required, and the runtime in seconds. Some results were aborted after one day.

| Instance   | $k$ | $D$ | $\tilde{\omega}_k$ | Nodes | Time | Nodes | Time |
|------------|-----|-----|---------------------|-------|------|-------|------|
| Erdos971   | 2   | 0.09| 42                  | 42    | 0.0  | 42    | 42   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.31| 117                 | 121   | 0.0  | 117   | 119  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.56| 235                 | 468   | 0.0  | 235   | 468  |
| Erdos972   | 2   | 0.01| 258                 | 258   | 0.7  | 258   | 258  |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.09| 517                 | 537   | 1.0  | 517   | 521  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.35| 1509               | $5.3 \times 10^7$ | 41811.3 | 1509 | 8197 | 6.4  |
| Erdos981   | 2   | 0.09| 43                  | 43    | 0.0  | 43    | 43   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.31| 123                 | 358   | 0.0  | 123   | 354  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.57| 245                 | 246   | 0.0  | 245   | 246  |
| Erdos982   | 2   | 0.01| 274                 | 274   | 0.8  | 274   | 274  |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.09| 547                 | 555   | 1.1  | 547   | 547  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.35| $\geq 1587$         | $1.2 \times 10^8$ | 1 day | 1594 | 618826 | 424.1 |
| Erdos991   | 2   | 0.09| 43                  | 44    | 0.0  | 43    | 44   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.31| 126                 | 375   | 0.0  | 126   | 374  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.57| 246                 | 491   | 0.0  | 246   | 491  |
| Erdos992   | 2   | 0.01| 277                 | 277   | 0.9  | 277   | 277  |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.09| 562                 | 573   | 1.2  | 562   | 562  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.35| $\geq 1636$         | $1.2 \times 10^8$ | 1 day | 1643 | 202543 | 145.6 |
| Erdos02    | 2   | 0.02| 508                 | 508   | 1.2  | 508   | 508  |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.20| 1014                | 1022  | 1.9  | 1014  | 1015 |
|            |     |     |                     |       |      |       |      |
|            | 4   | 1.00| 6927               | 6927  | 17.5 | 6927  | 6927 |
| c-fat200-1 | 2   | 0.13| 18                  | 41    | 0.0  | 18    | 35   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.19| 24                  | 74    | 0.0  | 24    | 48   |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.24| 30                  | 134   | 0.0  | 30    | 65   |
| c-fat200-2 | 2   | 0.27| 35                  | 35    | 0.0  | 35    | 35   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.39| 46                  | 488   | 0.0  | 46    | 102  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.50| 57                  | 1496  | 0.0  | 57    | 128  |
| c-fat200-5 | 2   | 0.71| 87                  | 11513 | 0.0  | 87    | 257  |
|            |     |     |                     |       |      |       |      |
|            | 3   | 1.00| 200                 | 200   | 0.0  | 200   | 200  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 1.00| 200                 | 200   | 0.0  | 200   | 200  |
| c-fat500-1 | 2   | 0.06| 21                  | 52    | 0.0  | 21    | 43   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.09| 28                  | 28    | 0.0  | 28    | 28   |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.11| 35                  | 35    | 0.0  | 35    | 35   |
| c-fat500-2 | 2   | 0.12| 39                  | 134   | 0.0  | 39    | 79   |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.17| 52                  | 52    | 0.0  | 52    | 52   |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.22| 65                  | 65    | 0.0  | 65    | 65   |
| c-fat500-5 | 2   | 0.31| 96                  | 10133 | 0.1  | 96    | 196  |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.44| 128                 | 128   | 0.0  | 128   | 128  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 0.56| $\geq 155$         | $2.1 \times 10^{10}$ | 1 day | 159 | 326 | 0.1 |
| c-fat500-10| 2   | 0.62| $\geq 187$         | $1.6 \times 10^{10}$ | 1 day | 189 | 560 | 0.1 |
|            |     |     |                     |       |      |       |      |
|            | 3   | 0.87| 252                 | 252   | 0.1  | 252   | 252  |
|            |     |     |                     |       |      |       |      |
|            | 4   | 1.00| 500                 | 500   | 0.1  | 500   | 500  |
| Instance  | $k$  | $D$  | $\tilde{\omega}_k$ | Nodes | Time | $\tilde{\omega}_k$ | Nodes | Time |
|-----------|------|------|---------------------|-------|------|---------------------|-------|------|
| p-hat300-1 | 2    | 1.00 | 299                | 299   | 0.0  | 299                | 299   | 0.0  |
|           | 3    | 1.00 | 300                | 300   | 0.0  | 300                | 300   | 0.0  |
|           | 4    | 1.00 | 10933              | 10933 | 0.0  | 10933              | 10933 | 0.0  |
| 3elt      | 2    | 0.00 | 10                 | 340   | 0.5  | 10                 | 340   | 0.5  |
|           | 3    | 0.01 | 16                 | 1582  | 0.5  | 16                 | 1582  | 1.1  |
|           | 4    | 0.01 | 37                 | 911   | 0.6  | 27                 | 911   | 0.8  |
| 4elt      | 2    | 0.00 | 11                 | 486   | 5.5  | 11                 | 486   | 7.5  |
|           | 3    | 0.01 | 20                 | 717   | 5.5  | 20                 | 717   | 8.3  |
|           | 4    | 0.01 | 36                 | 345   | 5.6  | 36                 | 345   | 6.1  |
| add20     | 2    | 0.04 | 124                | 124   | 0.1  | 124                | 124   | 0.2  |
|           | 3    | 0.25 | 671                | 671   | 0.3  | 671                | 671   | 0.3  |
|           | 4    | 0.67 | 1454               | 1454  | 0.7  | 1454               | 1454  | 0.7  |
| add32     | 2    | 0.00 | 32                 | 32    | 0.6  | 32                 | 32    | 0.6  |
|           | 3    | 0.01 | 99                 | 286   | 0.6  | 99                 | 286   | 0.6  |
|           | 4    | 0.03 | 268                | 268   | 0.6  | 268                | 268   | 0.6  |
| bcsstk29  | 2    | 0.01 | 72                 | 9752  | 5.4  | 72                 | 963   | 10.5 |
|           | 3    | 0.02 | 132               | $2.7\times10^5$ | 3141.2 | 132             | 7781  | 17.4 |
|           | 4    | 0.04 | $\geq 204$        | $3.7\times10^8$ | 1 day | 210              | 21689 | 27.8 |
| bcsstk30  | 2    | 0.01 | 219               | 224   | 19.9 | 219               | 219   | 20.5 |
|           | 3    | 0.03 | 496               | 509   | 23.3 | 496               | 496   | 24.3 |
|           | 4    | 0.05 | 843               | 854   | 29.2 | 843               | 845   | 30.8 |
| bcsstk31  | 2    | 0.00 | 189               | 189   | 29.0 | 189               | 189   | 30.2 |
|           | 3    | 0.01 | 278               | 605   | 30.4 | 278               | 369   | 32.0 |
|           | 4    | 0.03 | 428               | 119640 | 202.7 | 428             | 6588  | 48.1 |
| bcsstk33  | 2    | 0.03 | 141               | 141   | 2.1  | 141               | 141   | 2.1  |
|           | 3    | 0.08 | 228               | 26033 | 10.8 | 228               | 1744  | 5.8  |
|           | 4    | 0.15 | 435               | $2.0\times10^6$ | 825.1 | 435             | 52779 | 32.7 |
| crack     | 2    | 0.00 | 10                | 2894  | 2.4  | 10                | 2894  | 10.4 |
|           | 3    | 0.00 | 17                | 4996  | 2.5  | 17                | 4987  | 14.0 |
|           | 4    | 0.01 | 31                | 2173  | 2.6  | 31                | 2173  | 9.3  |
| cs4       | 2    | 0.00 | 6                 | 5780  | 11.4 | 6                 | 5780  | 97.8 |
|           | 3    | 0.00 | 12                | 7812  | 11.8 | 12                | 7812  | 109.6|
|           | 4    | 0.00 | 18                | 29032 | 13.6 | 18                | 29032 | 196.3|
| cti       | 2    | 0.00 | 7                 | 8918  | 6.6  | 7                 | 8918  | 84.1 |
|           | 3    | 0.00 | 15                | 6406  | 6.8  | 15                | 6406  | 60.2 |
|           | 4    | 0.01 | 26                | 62316 | 11.7 | 26                | 62316 | 162.3|
| data      | 2    | 0.01 | 18                | 638   | 0.2  | 18                | 617   | 0.3  |
|           | 3    | 0.02 | 32                | 4982  | 0.2  | 32                | 4913  | 0.4  |
|           | 4    | 0.04 | 52                | 40905 | 0.8  | 52                | 36089 | 0.9  |
| fe-4elt2  | 2    | 0.00 | 13                | 61    | 2.8  | 13                | 61    | 3.0  |
|           | 3    | 0.00 | 20                | 389   | 2.8  | 20                | 389   | 4.7  |
|           | 4    | 0.01 | 32                | 448   | 2.9  | 32                | 446   | 4.6  |
| fe-pwt    | 2    | 0.00 | 16                | 95    | 29.6 | 16                | 95    | 34.4 |
|           | 3    | 0.00 | 29                | 167   | 30.6 | 29                | 167   | 33.7 |
|           | 4    | 0.01 | 52                | 224   | 29.7 | 52                | 224   | 32.9 |
| Instance     | $k$ | $D$ | $\tilde{\omega}_k$ | Nodes | Time | $\tilde{\omega}_k$ | Nodes | Time |
|--------------|-----|-----|---------------------|-------|------|---------------------|-------|------|
| fe-sphere    | 2   | 0.00| 7                   | 14173 | 6.4  | 7                   | 14173 | 106.2|
|              | 3   | 0.00| 12                  | 34328 | 7.3  | 12                  | 34328 | 205.8|
|              | 4   | 0.00| 19                  | 73632 | 10.1 | 19                  | 73632 | 283.5|
| memplus      | 2   | 0.02| 574                 | 574   | 7.9  | 574                 | 574   | 7.8  |
|              | 3   | 0.26| 8057               | 8061  | 74.7 | 8057               | 8058  | 80.1 |
|              | 4   | 0.74| 8963               | 8963  | 106.0| 8963               | 8963  | 112.9|
| uk           | 2   | 0.00| 5                  | 433   | 0.5  | 5                   | 433   | 0.9  |
|              | 3   | 0.00| 8                  | 1891  | 0.5  | 8                   | 1891  | 1.4  |
|              | 4   | 0.01| 14                 | 2168  | 0.5  | 14                  | 2168  | 1.1  |
| vibrobox     | 2   | 0.02| 121                | 302   | 4.0  | 121                | 302   | 5.1  |
|              | 3   | 0.08| 408               | 1984  | 7.5  | 408               | 1984  | 12.0 |
|              | 4   | 0.26| 1094              | $8.8 \times 10^7$ | 1 day | $1094$ | $8.7 \times 10^7$ | 1 day |
| whitaker3    | 2   | 0.00| 9                 | 1222  | 2.3  | 9                  | 1222  | 7.3  |
|              | 3   | 0.00| 15               | 3724  | 2.3  | 15               | 3724  | 12.2 |
|              | 4   | 0.01| 23                | 6530  | 2.4  | 23                | 6530  | 14.8 |
| wing-nodal   | 2   | 0.02| 29                | 648   | 3.1  | 29                | 648   | 5.3  |
|              | 3   | 0.02| 54               | 13091 | 5.1  | 54               | 13091 | 23.6 |
|              | 4   | 0.04| 114              | $6.0 \times 10^7$ | $4639.0$ | $6.0 \times 10^7$ | $4676.0$ |
| adjnoun      | 2   | 0.50| 50                | 50    | 0.0  | 50                | 50    | 0.0  |
|              | 3   | 0.91| 83               | 164   | 0.0  | 83               | 164   | 0.0  |
|              | 4   | 0.99| 107              | 107   | 0.0  | 107              | 107   | 0.0  |
| as-22july06  | 2   | 0.04| 2391              | 2391  | 18.6 | 2391              | 2391  | 19.1 |
|              | 3   | 0.36| 8455              | 673880 | 13356.2 | 8455          | 94497 | 1834.0 |
|              | 4   | 0.79| 14911            | 14911 | 286.3| 14911            | 14911 | 288.8|
| astro-ph     | 2   | 0.01| 361              | 365   | 7.1  | 361              | 362   | 7.1  |
|              | 3   | 0.10| 1553             | 1567  | 16.8 | 1553             | 1560  | 20.1 |
|              | 4   | 0.35| 14911            | 14911 | 286.3| 14911            | 14911 | 288.8|
| celegans-meta| 2   | 0.44| 238             | 238   | 0.0  | 238             | 238   | 0.0  |
|              | 3   | 0.89| 371             | 371   | 0.0  | 371             | 371   | 0.0  |
|              | 4   | 0.98| 432             | 432   | 0.0  | 432             | 432   | 0.0  |
| celegansneural| 2   | 0.55| 135             | 135   | 0.0  | 135             | 135   | 0.0  |
|              | 3   | 0.95| 245             | 245   | 0.0  | 245             | 245   | 0.0  |
|              | 4   | 1.00| 295             | 295   | 0.0  | 295             | 295   | 0.0  |
| cond-mat     | 2   | 0.00| 108             | 108   | 6.5  | 108             | 108   | 6.8  |
|              | 3   | 0.01| 250             | 1403  | 7.8  | 250             | 844   | 7.7  |
|              | 4   | 0.05| 649             | $7.3 \times 10^7$ | 1 day | 720   | $6.7 \times 10^7$ | 823.3 |
| cond-mat-2003| 2   | 0.00| 203             | 204   | 22.7 | 203             | 204   | 22.6 |
|              | 3   | 0.02| $629$           | $6.5 \times 10^7$ | 1 day | $629$      | $6.2 \times 10^7$ | 1 day |
|              | 4   | 0.12| $2605$        | $1.8 \times 10^7$ | 1 day | $2606$   | $1.8 \times 10^7$ | 1 day |
| cond-mat-2005| 2   | 0.00| 279             | 279   | 37.8 | 279             | 279   | 39.0 |
|              | 3   | 0.03| $1060$          | $2.0 \times 10^7$ | 1 day | $1060$     | $1.9 \times 10^7$ | 1 day |
|              | 4   | 0.16| $4185$         | $6.2 \times 10^6$ | 1 day | $4185$    | $6.1 \times 10^6$ | 1 day |
| dolphins     | 2   | 0.32| 14              | 14    | 0.0  | 14               | 14    | 0.0  |
|              | 3   | 0.59| 30              | 30    | 0.0  | 30               | 30    | 0.0  |
|              | 4   | 0.77| 40              | 40    | 0.0  | 40               | 40    | 0.0  |
By comparing these results with the \( k \)-club results of Chang et al. [CHLS13], we see that in all but four cases the \( k \)-clique and \( k \)-club numbers are equal; all of these differences occur when \( k = 4 \). (Chang et al. did not investigate the “Erdos02” graph, but Wotzlaw [Wot14] confirmed privately that the \( k \)-clique and \( k \)-club numbers are the same here too.) On the other hand, the \( k \)-clique numbers are sometimes much easier to find, both algorithmically and computationally.

### Clique graphs
In the second part of Table 1, we present results from the “clique” graphs from the Second DIMACS implementation challenge\(^2\). These graphs were designed to test maximum clique implementations. Nearly all of these graphs have diameter 2, so a 2-clique covers the entire graph—we have ignored these. The only exceptions are the “c-fat” family (all of which are trivial for a maximum clique solver), and one of the “p\(\hat{h}\)” graphs.

With the domination rule, we solve all of these problems within a tenth of a second. Without, two of the results take over a day, and the rest remain trivial. Note that in several cases, for some values of \( k \)

\(^2\)http://dimacs.rutgers.edu/Challenges/
a $k$-clique covers the entire graph. Again using Chang et al.’s results [CHLS13], we see that for the first six graphs in this table the $k$-clique and $k$-club numbers are the same for each value of $k$ (Chang et al. did not investigate “c-fat500-10” or “p-hat300-1”).

**Partitioning graphs** The third part of Table 1 presents results from the smallest 20 partitioning graphs from the 10th DIMACS Implementation Challenge 3. Many of these graphs are considerably larger than those typically considered for the maximum clique problem, and we might expect our $O(|V|^2)$ memory requirements to cause problems. Nonetheless, with the domination rule there is only one instance which we were unable to solve within a day (and without the domination rule, there are two).

On the other hand, we sometimes see a significant cost where the domination rule does not help, and where the proof of optimality is not immediate: in “3elt” and “4elt”, our runtimes can nearly double, and for “cs4” and “cti” the slowdown is sometimes over a factor of ten. In other words, laziness does not help when the rule turns out to be used, but useless.

Five of these graphs were considered for the $k$-club problem by Wotzlaw [Wot14]. In all five cases, the $k$-clique and $k$-club numbers are the same for $k$ equal to 2, 3 and 4. However, the $k$-clique number was again consistently much easier to find.

**Clustering graphs** The final part of Table 1 presents results from the smallest 20 partitioning graphs from the 10th DIMACS Implementation Challenge 4. Again, from a maximum clique perspective these would be considered unusually large graphs. However, only five were unsolvable within a day (plus a sixth when the domination rule was not used), and half of the problems took under two seconds.

Seven of these graphs were considered for the $k$-club problem by Wotzlaw [Wot14]. In these cases, the 2-clique and 2-club numbers are the same, except for “football” where the 2-club number is 16 but the 2-clique number is 17; for $k = 3$ and $k = 4$ there are some differences. The difference in computational difficulty between the $k$-clique and $k$-club problems really stands out here: for “polblogs” with $k = 3$ and $k = 4$, Wotzlaw was unable to prove optimality within an hour, but we required less than a second to do so. In both of these cases the $k$-clique and $k$-club numbers are the same, which suggests a potential improvement to $k$-club algorithms: first solve the maximum $k$-clique problem instead, and test whether the result found is a $k$-club, before embarking upon a more complicated search. (Note that a negative result does not imply that the $k$-clique and $k$-club numbers necessarily differ, since solutions are not unique.)

### 3.2 Random Graphs

An Erdős-Rényi random graph $G(n, p)$ has $n$ vertices, and an edge between each distinct pair of vertices with probability $p$, chosen independently. Here we investigate the size of a maximum $k$-clique in such graphs, and the complexity of finding it. In each case, we use an average over 100 samples for every point. We do not use the domination rule for these experiments: the probability of random graphs having dominating vertices is very low.

In Figure 3 we illustrate the average value of $\tilde{\omega}_k$ in $G(200, p)$ for different values of $k$, and a range of values of $p$ for the $x$-axis. We see that even for very low edge probabilities, a maximum $k$-clique quickly covers the entire graph. (This is in contrast to the maximum clique problem, where a maximum clique does not even cover a quarter of the graph for edge probabilities below 0.75.) In Figure 3 we show the average size of the search space (number of nodes, or recursive calls made) for the same problem. We see that there is a complexity peak for each $k$, although the peak is much smaller for $k = 4$ than it is for $k = 3$, which is in turn much smaller than it is for $k = 2$. The peak also occurs for lower edge probabilities as $k$ increases. For contrast, for the maximum clique problem, the peak occurs at around edge probability 0.9, and is two orders of magnitude larger.

In Figures 5 and 6 we show the effect of changing $n$ and fixing $k = 2$. As $n$ increases from 50 to 200, the complexity peak becomes much more pronounced, and shifts slightly towards the left (lower edge probabilities).

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[http://staffweb.cms.gre.ac.uk/~wc06/partition/](http://staffweb.cms.gre.ac.uk/~wc06/partition/)  
[http://www.cc.gatech.edu/dimacs10/archive/clustering.shtml](http://www.cc.gatech.edu/dimacs10/archive/clustering.shtml)
Figure 3: Values of $\tilde{\omega}_k$ for random graphs $G(200, p)$, with varying edge probabilities. We see that even for very low edge probabilities, a maximum $k$-clique quickly covers the entire graph. This is in contrast to maximum cliques, which remain small even at much higher edge probabilities.

Figure 4: Search space size for random graphs $G(200, p)^k$, with varying edge probabilities. We see that 4-clique is easier than 3-clique in practice, which in turn is easier than 2-clique. (The complexity peak for maximum clique occurs at around edge probability 0.9, and requires approximately 15 million search nodes.)
Figure 5: The size of a maximum 2-clique in random graphs $G(n, p)$ with varying edge probabilities, and different values of $n$. For $G(50, p)$, a 2-clique has size average 50 from $p = 0.42$ onwards.

Figure 6: The search space size for the maximum 2-clique problem in random graphs $G(n, p)$ with varying edge probabilities, and for different values of $n$. As $n$ increases, the complexity peak grows and moves slowly to the left.
4 Conclusion

We have shown that using a maximum clique algorithm to solve the maximum $k$-clique algorithm for a graph $G$ by considering $G^k$ in place of $G$ is feasible in practice. This is despite $G^k$ potentially being dense even if $G$ is sparse.

We introduced a new lazy global domination rule. This was sometimes extremely beneficial—without this rule, we would have been unable to solve six of the problem instances we considered, and many others would have taken much longer. However, even with laziness there is still sometimes a cost to pay when this rule does nothing. This rule is thus harmful for the graphs typically considered for the maximum clique problem, and we see the benefit of tailoring algorithms to the problem being solved. We suggest that a similar rule may also be useful for the maximum $k$-club problem.

Quite often, we saw $k$-clique numbers and $k$-club numbers being the same. However, solving the maximum $k$-clique problem is much easier, both in terms of the algorithm and computationally. Thus it is worth checking whether the simpler model would be sufficient for practical applications before trying to solve the $k$-club problem.

In random graphs, we saw that $G(n, p)^k$ is easier than $G(n, p')$ with some higher probability $p'$. We also saw that as $k$ increases, the problem gets easier—this was not typically the case for some of the real world graphs.

Our results suggest that $k$ is a very coarse grained parameter. We saw that often a 2-clique or 3-clique would cover the entire graph. In these circumstances the increased restrictions for $k$-club are of no benefit. It is not obvious if somehow allowing a “fractional” value of $k$ could give more fine-grained control. Thus it may be worth considering other clique relaxations not based upon distance (although other models also have problems: a density-based relaxation known as quasi-clique, for example, can allow vertices with only a single edge to be added to a “clique” [ARS02]).

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