Fast Algorithms for the Maximum Clique Problem on Massive Sparse Graphs

Bharath Pattabiraman¹ [‡], Md. Mostofa Ali Patwary¹ [‡], Assefaw H. Gebremedhin², Wei-keng Liao¹, and Alok Choudhary¹ [‡] Authors contributed equally

Abstract. The maximum clique problem is a well known NP-Hard problem with applications in data mining, network analysis, information retrieval and many other areas related to the World Wide Web. There exist several algorithms for the problem with acceptable runtimes for certain classes of graphs, but many of them are infeasible for massive graphs. We present a new exact algorithm that employs novel pruning techniques and is able to quickly find maximum cliques in large sparse graphs. Extensive experiments on different kinds of synthetic and real-world graphs show that our new algorithm can be orders of magnitude faster than existing algorithms. We also present a heuristic that runs orders of magnitude faster than the exact algorithm while providing optimal or near-optimal solutions.

1 Introduction

A clique in an undirected graph is a subset of vertices in which every two vertices are adjacent to each other. The *maximum* clique problem seeks to find a clique of the largest possible size in a given graph.

The maximum clique problem, and the related *maximal* clique and clique *enumeration* problems, find applications in a wide variety of domains, many intimately related to the World Wide Web. A few examples include: information retrieval [2], community detection in networks [15, 29, 33], spatial data mining [40], data mining in bioinformatics [37], disease classification based on symptom correlation [7], pattern recognition [31], analysis of financial networks [5], computer vision [19], and coding theory [8]. To get a sense for how clique computation arises in the aforementioned contexts, consider a generic data mining or information retrieval problem. A typical objective here is to retrieve data that are considered similar based on some metric. Constructing a graph in which vertices correspond to data items and edges connect similar items, a clique in the graph would then give a cluster of similar data. More examples of application areas for clique problems can be found in [18, 30].

The maximum clique problem is NP-Hard [16]. Most exact algorithms for solving it employ some form of *branch-and-bound* approach. While branching systematically searches for all candidate solutions, bounding (also known as *pruning*) discards fruitless candidates based on a previously computed bound. The algorithm of Carraghan

and Pardalos [9] is an early example of a simple and effective branch-and-bound algorithm for the maximum clique problem. More recently, Östergård [28] introduced an improved algorithm and demonstrated its relative advantages via computational experiments. Tomita and Seki [35], and later, Konc and Janežič [21] use upper bounds computed using vertex coloring to enhance the branch-and-bound approach. Other examples of branch-and-bound algorithms for the clique problem include [6, 34, 3]. Prosser [32] in a recent work compares various exact algorithms for the maximum clique problem.

In this paper, we present a new exact branch-and-bound algorithm for the maximum clique problem that employs several new pruning strategies in addition to those used in [9], [28], [35] and [21], making it suitable for massive graphs. We run our algorithms on a large variety of test graphs and compare its performance with the algorithm of Carraghan and Pardalos [9], the algorithm of Östergård [28] and the algorithm of Konc and Janežič [21]. We find our new exact algorithm to be up to orders of magnitude faster on large, sparse graphs and of comparable runtime on denser graphs. We also present a hew heuristic, which runs several orders of magnitude faster than the exact algorithm while providing solutions that are optimal or near-optimal for most cases. We have made our implementations publicly available³. Both the exact algorithm and the heuristic are well-suited for parallelization.

2 Related Previous Algorithms

Given a simple undirected graph G, the maximum clique can clearly be obtained by enumerating all of the cliques present in it and picking the largest of them. Carraghan and Pardalos [9] introduced a simple-to-implement algorithm that avoids enumerating all cliques and instead works with a significantly reduced partial enumeration. The reduction in enumeration is achieved via a pruning strategy which reduces the search space tremendously. The algorithm works by performing at each step i, a depth first search from vertex v_i , where the goal is to find the largest clique containing the vertex v_i . At each depth of the search, the algorithm compares the number of remaining vertices that could potentially constitute a clique containing vertex v_i against the size of the largest clique encountered thus far. If that number is found to be smaller, the algorithm backtracks (search is pruned).

Östergård [28] devised an algorithm that incorporated an additional pruning strategy to the one by Carraghan and Pardalos. The opportunity for the new pruning strategy is created by *reversing* the order in which the search is done by the Carraghan-Pardalos algorithm. This allows for an additional pruning with the help of some auxiliary book-keeping. Experimental results in [28] showed that the Östergård algorithm is faster than the Carraghan-Pardalos algorithm on random and DIMACS benchmark graphs [20]. However, the new pruning strategy used in this algorithm is intimately tied to the order in which vertices are processed, introducing an inherent sequentiality into the algorithm.

A number of existing branch-and-bound algorithms for maximum clique also use a vertex-coloring of the graph to obtain an upper bound on the maximum clique. A popular and recent algorithm based on this idea is the algorithm of Tomita and Seiku

http://cucis.ece.northwestern.edu/projects/MAXCLIQUE/

[35] (known as MCQ). More recently, Konc and Janežič [21] presented an improved version of MCQ, known as MaxCliqueDyn (MCQD and MCQD+CS), that involves the use of tighter, computationally more expensive upper bounds applied on a fraction of the search space.

3 The New Algorithms

We describe in this section new algorithms that overcome the shortcomings mentioned earlier; the new algorithms use additional pruning strategies, maintain simplicity, and avoid a sequential computational order. We begin by first introducing the following notations. We identify the n vertices of the input graph G = (V, E) as $\{v_1, v_2, \ldots, v_n\}$. The set of vertices adjacent to a vertex v_i , the set of its neighbors, is denoted by $N(v_i)$. And the degree of the vertex v_i , the cardinality of $N(v_i)$, is denoted by $d(v_i)$.

3.1 The Exact Algorithm

The maximum clique in a graph can be found by computing the largest clique containing each vertex and picking the largest among these. A key element of our exact algorithm is that during the search for the largest clique containing a given vertex, vertices that cannot form cliques larger than the current maximum clique are pruned, in a hierarchical fashion. The method is outlined in detail in Algorithm 1. Throughout, the variable max stores the size of the maximum clique found thus far. Initially it is set to be equal to the lower bound lb provided as an input parameter. It gives the maximum clique size when the algorithm terminates.

To obtain the largest clique containing a vertex v_i , it is sufficient to consider only the neighbors of v_i . The main routine MAXCLIQUE thus generates for each vertex $v_i \in V$ a set $U \subseteq$

Algorithm 1 Algorithm for finding the maximum clique of a given graph. *Input*: Graph G = (V, E), lower bound on clique lb (default, 0). *Output*: Size of maximum clique.

```
1: procedure MAXCLIQUE(G = (V, E), lb)
2:
         max \leftarrow lb
3:
         for i:1 to n do
4:
             if d(v_i) \geq max then
                                                    ⊳ Pruning 1
5:
                  U \leftarrow \emptyset
6:
                 for each v_i \in N(v_i) do
7:
                     if j > i then
                                                    ⊳ Pruning 2
 8:
                          if d(v_i) \geq max then \triangleright Pruning 3
9:
                              U \leftarrow U \cup \{v_j\}
10:
                  CLIQUE(G, U, 1)
– Subroutine
```

if $U = \emptyset$ then 3: if size > max then 4: $max \leftarrow size$ 5: return while |U| > 0 do 6: 7: if $size + |U| \le max$ then ⊳ Pruning 4 8: return 9: Select any vertex u from U10: $U \leftarrow U \setminus \{u\}$ $N'(u) := \{w | w \in N(u) \land d(w) \ge max\} \triangleright$ Pruning 5 $CLIQUE(G, U \cap N'(u), size + 1)$ 12:

1: **procedure** CLIQUE(G = (V, E), U, size)

 $N(v_i)$ (neighbors of v_i that survive pruning) and calls the subroutine CLIQUE on U. The subroutine CLIQUE goes through every relevant clique containing v_i in a recursive fashion and returns the largest. We use size to maintain the size of the clique found

at any point through the recursion. Since we start with a clique of just one vertex, the value of *size* is set to one initially, when CLIQUE is called (Line 10, MAXCLIQUE).

Our algorithm consists of several pruning steps. Pruning 1 (Line 4, MAXCLIQUE) filters vertices having strictly fewer neighbors than the size of the maximum clique already computed. These vertices can be ignored, since even if a clique were to be found, its size would not be larger than max. While forming the neighbor list U for a vertex v_i , we include only those of v_i 's neighbors for which the largest clique containing them has not been found (Pruning 2; Line 7, MAXCLIQUE), to avoid recomputing previously found cliques. Pruning 3 (Line 8, MAXCLIQUE) excludes vertices $v_j \in N(v_i)$ that have degree less than the current value of max, since any such vertex could not form a clique of size larger than max. Pruning 4 (Line 7, CLIQUE) checks for the case where even if all vertices of U were added to get a clique, its size would not exceed that of the largest clique encountered so far in the search, max. Pruning 5 (Line 11, CLIQUE) reduces the number of comparisons needed to generate the intersection set in Line 12. Note that the routine CLIQUE is similar to the Carraghan-Pardalos algorithm [9]; Pruning 5 accounts for the main difference. Also, Pruning 4 is used in most existing algorithms, whereas Prunings 1, 2, 3 and 5 are not.

3.2 The Heuristic

The exact algorithm examines all relevant cliques containing every vertex. Our heuristic, shown in Algorithm 2, considers only the *maximum degree* neighbor at each step instead of recursively considering all neighbors from the set U, and thus is much faster.

3.3 Complexity

The exact algorithm, Algorithm 1, examines for every vertex v_i all candidate cliques containing the vertex v_i in its search for the largest clique. Its time complexity is exponential in the worst case. The heuristic, Algorithm 2, loops over the n vertices, each time possibly calling the subroutine CLIQUEHEU, which effectively is a loop that runs until the

Algorithm 2 Heuristic for finding the maximum clique in a graph. *Input*: Graph G=(V,E). *Output*: Approximate size of maximum clique.

```
1: procedure MAXCLIQUEHEU(G = (V, E))

2: for i: 1 to n do

3: if d(v_i) \ge max then

4: U \leftarrow \emptyset

5: for each v_j \in N(v_i) do

6: if d(v_j) \ge max then

7: U \leftarrow U \cup \{v_j\}

8: CLIQUEHEU(G, U, 1)
```

Subroutine

```
1: procedure CLIQUEHEU(G = (V, E), U, size)
2:
       if U = \emptyset then
3:
           if size > max then
4:
               max \leftarrow size
5:
           return
6:
       Select a vertex u \in U of maximum degree in G
       U \leftarrow U \setminus \{u\}
8:
       N'(u) := \{w | w \in N(u) \land d(w) \ge max\}
9:
       CLIQUEHEU(G, U \cap N'(u), size + 1)
```

set U is empty. Clearly, |U| is bounded by the max degree Δ in the graph. The subroutine also includes the computation of a neighbor list, whose runtime is bounded by $O(\Delta)$. Thus, the time complexity of the heuristic is bounded by $O(n \cdot \Delta^2)$.

Table 1. Overview of real-world graphs in the testbed and their origins.

Graph	Description
cond-mat-2003 [26]	A collaboration network of scientists posting preprints on
	the condensed matter archive at www.arxiv.org in the period
email-Enron [23]	A communication network representing email exchanges.
dictionary28 [4]	Pajek network of words.
Fault_639 [14]	A structural problem discretizing a faulted gas reservoir with
	tetrahedral Finite Elements and triangular Interface Elements.
audikw_1 [11]	An automotive crankshaft model of TETRA elements.
bone010 [39]	A detailed micro-finite element model of bones representing
	the porous bone micro-architecture.
af_shell [11]	A sheet metal forming simulation network.
as-Skitter [23]	An Internet topology graph from trace routes run daily in 2005.
roadNet-CA [23]	A road network of California. Nodes represent intersections
	and endpoints and edges represent the roads connecting them.
kkt_power [11]	An Optimal Power Flow (nonlinear optimization) network.

4 Experiments and Results

We present in this section results comparing the performance of our algorithm with the algorithms of Carraghan-Pardalos [9], Östergård algorithm [28], and Konc and Janezik [21]. We implemented the algorithm of [9] ourselves. For the algorithm of [28], we used the publicly available *cliquer* source code [27]. For the algorithm of [21], we used the code *MaxCliqueDyn* (MCQD, available at http://www.sicmm.org/~konc/maxclique/). Among the variants available in MCQD, we report results on MCQD+CS (which uses improved coloring and dynamic sorting), since it is the best-performing variant.

The experiments are performed on a Linux workstation running 64-bit Red Hat Enterprise Linux Server release 6.2 with a 2 GHz Intel Xeon E7540 processor. The codes are implemented in C++ and compiled using gcc version 4.4.6 with -O3 optimization.

4.1 Test Graphs

Our testbed is grouped in three categories.

- 1. Real-world graphs Under this category, we consider 10 graphs (downloaded from the University of Florida Sparse Matrix Collection [11]) that originate from various real-world applications. Table 1 gives a quick overview of the graphs and their origins.
- 2. Synthetic Graphs In this category we consider 15 graphs generated using the R-MAT algorithm [10]. The graphs are subdivided in three categories depending on the structures they represent.
- **A. Random graphs** (5 graphs) Erdős-Rényi random graphs generated using R-MAT with the parameters (0.25, 0.25, 0.25, 0.25). Denoted with prefix *rmat_er*.
- **B. Skewed Degree, Type 1 graphs** (5 graphs) graphs generated using R-MAT with the parameters (0.45, 0.15, 0.15, 0.25). Denoted with prefix *rmat_sd1*.
- **C. Skewed Degree, Type 2 graphs** (5 graphs) graphs generated using R-MAT with the parameters (0.55, 0.15, 0.15, 0.15). Denoted with prefix *rmat_sd2*.

Table 2. Structural properties (the number of vertices, |V|; edges, |E|; and the maximum degree, Δ) of the graphs, G in the testbed: DIMACS Challenge graphs (upper left); UF Collection (lower and middle left); RMAT graphs (right).

\overline{G}	V	E	Δ	G	V	E	Δ
cond-mat-2003	31,163	120,029	202	rmat_sd1_1	131,072	1,046,384	407
email-Enron	36,692	183,831	1,383	rmat_sd1_2	262,144	2,093,552	558
dictionary28	52,652	89,038	38	rmat_sd1_3	524,288	4,190,376	618
Fault_639	638,802	13,987,881	317	rmat_sd1_4	1,048,576	8,382,821	802
audikw_I	943,695	38,354,076	344	rmat_sd1_5	2,097,152	16,767,728	1,069
bone010	986,703	35,339,811	80	rmat_sd2_1	131,072	1,032,634	2,980
af_shell10	1,508,065	25,582,130	34	rmat_sd2_2	262,144	2,067,860	4,493
as-Skitter	1,696,415	11,095,298	35,455	rmat_sd2_3	524,288	4,153,043	6,342
roadNet-CA	1,971,281	2,766,607	12	rmat_sd2_4	1,048,576	8,318,004	9,453
kkt_power	2,063,494	6,482,320	95	rmat_sd2_5	2,097,152	16,645,183	14,066
rmat_er_1	131,072	1,048,515	82	hamming6-4	64	704	22
$rmat_er_2$	262,144	2,097,104	98	johnson8-4-4	70	1,855	53
rmat_er_3	524,288	4,194,254	94	keller4	171	9,435	124
rmat_er_4	1,048,576	8,388,540	97	c-fat200-5	200	8,473	86
rmat_er_5	2,097,152	16,777,139	102	brock200_2	200	9,876	114

3. DIMACS graphs This last category consists of 5 graphs selected from the Second DIMACS Implementation Challenge [20].

The DIMACS graphs are an established benchmark for the maximum clique problem, but they are of rather limited size and variation. In contrast, the real-work networks included in category 1 of the testset and the synthetic (RMAT) graphs in category 2 represent a wide spectrum of large graphs posing varying degrees of difficulty for testing the algorithms. The *rmat_er* graphs have *normal* degree distribution, whereas the *rmat_sd1* and *rmat_sd2* graphs have skewed degree distributions and contain many dense local subgraphs. The *rmat_sd1* and *rmat_sd2* graphs differ primarily in the magnitude of maximum vertex degree they contain; the *rmat_sd2* graphs have much higher maximum degree. Table 2 lists basic structural information (the number of vertices, number of edges and the maximum degree) about all 30 of the test graphs.

4.2 Results

Table 3 shows the size of the maximum clique (ω) and the runtimes of our exact algorithm (Algorithm 1) and the algorithms of Caraghan and Pardalos (CP), Östergård (*cliquer*) and Konc and Janežič (MCQD+CS) for all the graphs in the testbed. The last two columns show the results of our heuristic (Algorithm 2)—the size of the maximum clique returned and its runtime. The columns labeled P1, P2, P3 and P5 list the number of vertices/branches pruned in the respective pruning steps of Algorithm 1. Pruning 4 is omitted since it is used by all the algorithms compared in the table. These numbers have been rounded (K stands for 10^3 , M for 10^6 and B for 10^9), although the exact numbers can be found in the Appendix (Table 4).

In Table 3, the fastest runtime for each instance is indicated with boldface. An asterisk (*) indicates that an algorithm did not terminate within 25,000 seconds for a

Table 3. Comparison of runtimes (in seconds) of algorithms [9] (*CP*), [28] (*cliquer*), [21] (*MCQD+CS*) and our new exact algorithm (τ_{A1}) for the graphs in the testbed. *P1*, *P2*, *P3* and *P5* are the number of vertices/branches pruned in steps Pruning 1, 2, 3 and 5 of our exact algorithm (K stands for 10^3 , M for 10^6 and B for 10^9). ω denotes the maximum clique size in the graph, ω_{A2} denotes the clique size returned by our heuristic and τ_{A2} shows its runtime.

				τ_{MCQD}							
Graph	ω	τ_{CP}	$ au_{cliquer}$	+CS	$ au_{A1}$	P1	P2	P3	P5	ω_{A2}	$ au_{A2}$
cond-mat-2003	25	4.875	11.17	2.41	0.011	29K	48K	6,527	17K	25	< 0.01
email-Enron	20	7.005	15.08	3.70	0.998			4,060	8M	18	0.261
dictionary28	26	7.700	32.74	7.69	< 0.01	52K	4,353	2,114	107	26	< 0.01
Fault_639	18	14571.20	4437.14	-	20.03	36	13M	126		18	5.80
audikw_1	36	*	9282.49	-	190.17	4,101	38M	59K	721K	36	58.38
bone010	24	*	10002.67	-	393.11	37K	34M	361K	44M	24	24.39
af_shell10	15	*	21669.96	-	50.99	19	25M	75	2,105	15	10.67
as-Skitter	67	24385.73	*	-	3838.36	1M	6M	981K	737M	66	27.08
roadNet-CA	4	*	*	-	0.44	1M	1M	370K	4,302	4	0.08
kkt_power	11	*	*	-	2.26	1M	4M	401K	2M	11	1.83
rmat_er_1	3	256.37	215.18	49.79	0.38	780	1M	915	8,722	3	0.12
rmat_er_2	3	1016.70	865.18	_	0.78	2.019	2M	2,351	23K	3	0.24
rmat_er_3	3	4117.35	3456.39	_	1.87	4,349	4M	4,960	50K	3	0.49
rmat_er_4	3	16419.80	13894.52	_	4.16	9,032	8M	10K	106K	3	1.44
rmat_er_5	3	*	*	-	9.87	18K	16M	20K	212K	3	2.57
rmat_sd1_1	6	225.93	214.99	50.08	1.39	39K	1M	23K	542K	6	0.45
rmat_sd1_2	6	912.44	858.80	-	3.79	90K	2M	56K	1M	6	0.98
rmat_sd1_3	6	3676.14	3446.02	_	8.17	176K	4M	106K	2M	6	1.78
rmat_sd1_4	6	14650.40	13923.93	_	25.61	369K		214K	5M	6	4.05
rmat_sd1_5	6	*	*	-	46.89	777K		455K	12M	6	9.39
rmat_sd2_1	26	427.41	213.23	48.17	242.20	110K	853K	88K	614M	26	32.83
rmat_sd2_2	35	4663.62	851.84	-	3936.55	232K		195K	1B	35	95.89
rmat_sd2_3	39	13626.23	3411.14	_	10647.84	470K	3M		1B	37	245.51
rmat_sd2_4	43	*	13709.52	_	*	*	*	*	*	42	700.05
rmat_sd2_5	N	*	*	-	*	*	*	*	*	51	1983.21
hamming6-4	4	< 0.01	< 0.01	< 0.01	< 0.01	0	704	0	0	4	< 0.01
johnson8-4-4	14	0.19	< 0.01	< 0.01	0.23	0	1,855	0	0	14	< 0.01
keller4	11	22.19	0.15	0.02	23.35			0	0	11	< 0.01
c-fat200-5	58	0.60	0.13	0.02	0.93		8,473	0	0	58	0.04
brock200_2	12	0.98	0.02	< 0.01	1.10		9,876	0	0	10	< 0.01
		1				1				1	

particular instance. A hyphen (-) indicates that the publicly available implementation (the *MaxCliqueDyn* code) had to be aborted because the input graph was too large for the implementation to handle. Even for the instances for which the code eventually run successfully, we had to first modify the graph reader to make it able to handle graphs with multiple connected components. For the graph *rmat_sd2_5*, none of the algorithms computed the maximum clique size in a reasonable time; the entry there is marked with N, standing for "Not Known".

We discuss in what follows our observations from this table for the exact algorithm and the heuristic.

Exact algorithms As expected, our exact algorithm gave the same size of maximum clique as the other three algorithms for all test cases. In terms of runtime, its relative performance compared to the other three varied in accordance with the advantages afforded by the various pruning steps.

Vertices that are discarded by Pruning 1 are skipped in the main loop of the algorithm, and the largest cliques containing them are not computed. Pruning 2 avoids re-computing previously computed cliques in the neighborhood of a vertex. In the absence of Pruning 1, the number of vertices pruned by Pruning 2 would be bounded by the number of edges in the graph (note that this is more than the total number of vertices in the graph). While Pruning 3 reduces the size of the input set on which the maximum clique is to be computed, Pruning 5 brings down the time taken to generate the intersection set in Line 12 of the subroutine. Pruning 4 corresponds to back tracking. Unlike Pruning steps 1, 2, 3 and 5, Pruning 4 is used by all three of the other algorithms in our comparison. The primary strength of our algorithm is its ability to take advantage of pruning in multiple steps in a hierarchical fashion, allowing for opportunities for one or more of the steps to kick in and impact performance.

As a result of the differences seen in the effects of the pruning steps, as discussed below, the runtime performance of our algorithm (seen in Table 3) compared to the other three algorithms varied in accordance with the difference in the structures represented by the different categories of graphs in the testbed.

Real-world Graphs. For most of the graphs in this category, it can be seen that our algorithm runs several orders of magnitude faster than the other three, mainly due to the large amount of pruning the algorithm enforced. These numbers also illustrate the great benefit of hierarchical pruning. For the graphs *Fault_639*, *audikw_1* and *af_shell10*, there is only minimal impact by Prunings 1, 3 and 5, whereas Pruning 2 makes a big difference resulting in impressive runtimes. The number of vertices pruned in steps Pruning 1 and 3 varied among the graph *within* the category, ranging from 0.001% for *af_shell* to a staggering 97% for *as-Skitter* for the step Pruning 1.

Synthetic Graphs. For the synthetic graph types *rmat_er* and *rmat_sd1*, our algorithm clearly outperforms the other three by a few orders of magnitude in all cases. This is also primary due to the high number of vertices discarded by the new pruning steps. In particular, for *rmat_sd1* graphs, between 30 to 37% of the vertices are pruned just in the step Pruning 1. For the *rmat_sd2* graphs, which have relatively larger maximum clique and higher maximum degree than the *rmat_sd1* graphs, our algorithm is observed to be faster than CP but slower than *cliquer*.

DIMACS Graphs. The runtime of our exact algorithm for the DIMACS graphs is in most cases comparable to that of CP and higher than that of *cliquer* and *MCQD+CS*. For these graphs, only Pruning 2 was found to be effective, and thus the performance results agree with one's expectation. We include in the Appendix timing results on a larger collection of DIMACS graphs.

It is to be noted that the DIMACS graphs are intended to serve as challenging test cases for the maximum clique problem, and graphs with such high edge densities and low vertex count are rare in practice. Most of these have between 20 to 1024 vertices with an average edge density of roughly 0.6, whereas, most real world graphs are often very large and sparse. Good examples are Internet topology graphs [13], the web graph [22], social network graphs [12], and the real-world graphs in our testbed.

The Heuristic It can be seen that our heuristic runs several orders of magnitude faster than our exact algorithm, while delivering either optimal or very close to optimal solution. It gave the optimal solution on 25 out of the 30 test cases. On the remaining 5 cases where it was suboptimal, its accuracy ranges from 83% to 99% (on average 93%). Additionally, we run the heuristic by choosing a vertex randomly in Line 6 of Algorithm 2 instead of the one with the maximum degree. We observe that on average, the solution is optimal only for less than 40% of the test cases compared to 83% when selecting the maximum degree vertex.

Figure 1 provides an aggregated visual summary of the runtime trends of the various algorithms across the five categories of graphs in the testbed.

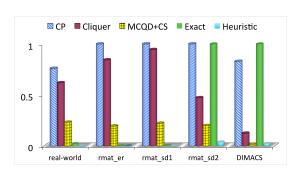


Fig. 1. Runtime (normalized, mean) comparison between various algorithms. For each category of graph, first, all runtimes for each graph were normalized by the runtime of the slowest algorithm for that graph, and then the mean was calculated for each algorithm. Graphs were considered only if the runtimes for at least three algorithms was less than the 25,000 seconds limit set.

To give a sense of runtime growth rates, we provide in Figure 2 plots of the runtime of the new exact algorithm and the heuristic for the synthetic and real-world graphs in the testbed. Besides the curves corresponding to the runtimes of the *exact* algorithm and the *heuristic*, the figures also include a curve corresponding to the number of *edges* in the graph divided by the clock frequency of the computing platform used in the experiment. This curve is added to facilitate comparison between the growth rate of the algorithms with that of a linear-time (in the size of the graph) growth rate. It can be seen that the runtime of the heuristic by and large grows somewhat linearly with the size of a graph. The exact algorithm's runtime, which is orders of magnitude larger than the heuristic, exhibited a similar growth behavior for these test-cases (even though its worst-case complexity suggests exponential growth).

5 Conclusion

We presented a new exact and a new heuristic algorithm for the maximum clique problem. We performed extensive experiments on three broad categories of graphs comparing the performance of our algorithms to the algorithms due to Carraghan and Pardalos (CP) [9], Östergård (*cliquer*) [28] and Konc and Janežič (MCQD+CS) [21]. For DI-MACS benchmark graphs and certain dense synthetic graphs ($rmat_sd2$), our new exact algorithm performs comparably with the CP algorithm, but slower than *cliquer* and MCQD+CS. For large sparse graphs, both synthetic and real-world, our new algorithm runs several orders of magnitude faster than the other three. The heuristic, which runs many orders of magnitude faster than our exact algorithm and the others, gave opti-

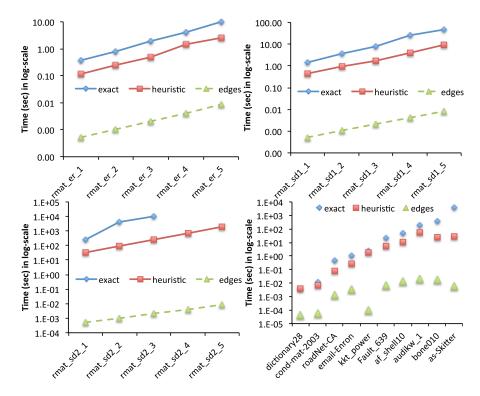


Fig. 2. Run time plots of the new exact and heuristic algorithms. The third curve, labeled *edges*, shows the quantity, number of edges in the graph divided by the clock frequency of the computing platform used in the experiment.

mal solution for 83% of the test cases, and when it is sub-optimal, its accuracy ranged between 0.83 and 0.99.

In this work, we did not compare the performance of our algorithm against those for which an implementation is not publicly available such as [36,25]. It would be interesting to implement these and compare in future work. Further, the MCQD implementation uses an adjacency matrix, whereas our algorithm uses an adjacency list to represent the graph. Although it is unlikely for the overall results to be drastically different with a change in the graph representation, it will be interesting to study to what degree the performance will change with the change in graph representation. The heuristic's performance is impressive as presented; still it is worthwhile to compare with other existing heuristics approaches such as [1, 17].

Acknowledgements

This work is supported in part by the following grants: NSF awards CCF-0833131, CNS-0830927, IIS-0905205, CCF-0938000, CCF-1029166, and OCI-1144061; DOE awards DE-FG02-08ER25848, DE-SC0001283, DE-SC0005309, DESC0005340, and

DESC0007456; AFOSR award FA9550-12-1-0458. The work of Assefaw Gebremedhin is supported by the NSF award CCF-1218916 and by the DOE award DE-SC0010205.

References

- 1. D. Andrade, M. Resende, and R. Werneck, *Fast local search for the maximum independent set problem*, Journal of Heuristics, 18 (2012), pp. 525–547.
- J.G. Augustson and J. Minker, An analysis of some graph theoretical cluster techniques, J. ACM 17 (1970), pp. 571–588.
- 3. L. Babel and G. Tinhofer, *A branch and bound algorithm for the maximum clique problem*, Mathematical Methods of Operations Research 34 (1990), pp. 207–217.
- V. Batagelj and A. Mrvar, Pajek datasets (2006), URL http://vlado.fmf.uni-lj. si/pub/networks/data/.
- V. Boginski, S. Butenko, and P.M. Pardalos, Statistical analysis of financial networks, Computational Statistics & Data Analysis 48 (2005), pp. 431–443.
- 6. I.M. Bomze, M. Budinich, P.M. Pardalos, and M. Pelillo, *The Maximum Clique Problem*, in *Handbook of Combinatorial Optimization*, Kluwer Academic Publishers, 1999, pp. 1–74.
- 7. R.E. Bonner, On some clustering techniques, IBM J. Res. Dev. 8 (1964), pp. 22–32.
- 8. A.E. Brouwer, J.B. Shearer, N.J.A. Sloane, and W.D. Smith, *A new table of constant weight codes.*, IEEE Transactions on Information Theory (1990), pp. 1334–1380.
- R. Carraghan and P. Pardalos, An exact algorithm for the maximum clique problem, Oper. Res. Lett. 9 (1990), pp. 375–382.
- 10. D. Chakrabarti and C. Faloutsos, *Graph mining: Laws, generators, and algorithms*, ACM Comput. Surv. 38 (2006).
- 11. T.A. Davis and Y. Hu, *The university of florida sparse matrix collection*, ACM Transactions on Mathematical Software (TOMS) 38 (2011), pp. 1:1–1:25.
- 12. P. Domingos and M. Richardson, *Mining the network value of customers*, in *Proc. of the 7th ACM SIGKDD KDD'01*, KDD '01, San Francisco, California, ACM, New York, NY, USA, 2001, pp. 57–66.
- 13. M. Faloutsos, P. Faloutsos, and C. Faloutsos, On power-law relationships of the Internet topology, in Proc. of the conference on Applications, technologies, architectures, and protocols for computer communication, SIGCOMM '99, Cambridge, Massachusetts, United States, ACM, 1999, pp. 251–262.
- 14. M. Ferronato, C. Janna, G. Gambolati, *Mixed constraint preconditioning in computational contact mechanics*, Computer Methods in Applied Mechanics and Engineering 197 (2008), pp. 3922 3931.
- 15. S. Fortunato, Community detection in graphs, Physics Reports 486 (2010), pp. 75–174.
- 16. M.R. Garey and D.S. Johnson, W. H. Freeman & Co., New York, NY, USA 1979.
- 17. A. Grosso, M. Locatelli, and W. Pullan, *Simple ingredients leading to very efficient heuristics for the maximum clique problem*, Journal of Heuristics, 14 (2008), pp. 587–612.
- 18. G. Gutin, Gross, J. L.; Yellen, J., Handbook of graph theory, Discrete Mathematics & Its Applications, CRC Press 2004.
- 19. R. Horaud and T. Skordas, *Stereo correspondence through feature grouping and maximal cliques*, IEEE Trans. Pattern Anal. Mach. Intell. 11 (1989), pp. 1168–1180.
- D. Johnson and M.A. Trick, Editors, Cliques, coloring and satisfiability: Second dimacs implementation challenge, DIMACS Series on Discrete Mathematics and Theoretical Computer Science 26 (1996).
- 21. J. Konc and D. Janežič, *An improved branch and bound algorithm for the maximum clique problem*, MATCH Commun. Math. Comput. Chem., 2007, 58, pp. 569590.

- 22. R. Kumar, P. Raghavan, S. Rajagopalan, and A. Tomkins, *Extracting Large-Scale Knowledge Bases from the Web.*, in *VLDB* '99, 1999, pp. 639–650.
- J. Leskovec, J. Kleinberg, and C. Faloutsos, Graphs over time: densification laws, shrinking diameters and possible explanations, in Proceedings of the eleventh ACM SIGKDD international conference on Knowledge discovery in data mining, KDD '05, Chicago, Illinois, USA, ACM, New York, NY, USA, 2005, pp. 177–187.
- 24. L. Leydesdorff, On the normalization and visualization of author co-citation data: Salton's cosine versus the jaccard index, J. Am. Soc. Inf. Sci. Technol. 59 (2008), pp. 77–85.
- 25. C.-M. Li and Z. Quan, An efficient branch-and-bound algorithm based on massat for the maximum clique problem, 2010.
- M.E.J. Newman, Coauthorship networks and patterns of scientific collaboration, Proceedings of the National Academy of Sciences of the United States of America 101 (2004), pp. 5200–5205.
- 27. S. Niskanen and P.R.J. Östergård, *Cliquer user's guide, version 1.0*, Tech. Rep. T48, Communications Laboratory, Helsinki University of Technology, Espoo, Finland, 2003.
- 28. P.R.J. Östergård, *A fast algorithm for the maximum clique problem*, Discrete Appl. Math. 120 (2002), pp. 197–207.
- 29. G. Palla, I. Derenyi, I. Farkas, and T. Vicsek, *Uncovering the overlapping community structure of complex networks in nature and society*, Nature 435 (2005), pp. 814–818.
- P.M. Pardalos and J. Xue, *The maximum clique problem*, Journal of Global Optimization 4 (1994), pp. 301–328.
- 31. M. Pavan and M. Pelillo, A new graph-theoretic approach to clustering and segmentation, in *Proc. of the 2003 IEEE computer society conference on Computer vision and pattern recognition*, CVPR'03, Madison, Wisconsin, IEEE Computer Society, Washington, DC, USA, 2003, pp. 145–152.
- 32. P. Prosser, Exact algorithms for maximum clique: A computational study, arXiv preprint arXiv:1207.4616v1 (2012).
- 33. S. Sadi, S. Öğüdücü, and A.S. Uyar, An efficient community detection method using parallel clique-finding ants, in Proc. of IEEE Congress on Evol. Comp, July, 2010, pp. 1–7.
- 34. P. San Segundo, D. Rodríguez-Losada, and A. Jiménez, *An exact bit-parallel algorithm for the maximum clique problem*, Comput. Oper. Res. 38 (2011), pp. 571–581.
- 35. E. Tomita and T. Seki, An efficient branch-and-bound algorithm for finding a maximum clique, in Proc. of the 4th international conference on Discrete mathematics and theoretical computer science, Dijon, France, Springer-Verlag, Berlin, Heidelberg, 2003, pp. 278–289.
- 36. E. Tomita, Y. Sutani, T. Higashi, S. Takahashi, and M. Wakatsuki, A simple and faster branch-and-bound algorithm for finding a maximum clique, in WALCOM: Algorithms and Computation, M. Rahman and S. Fujita, eds., vol. 5942 of Lecture Notes in Computer Science, Springer Berlin Heidelberg, 2010, pp. 191–203.
- 37. T. Matsunaga, C. Yonemori, E. Tomita, and M. Muramatsu, *Clique-based data mining for related genes in a biomedical database*, BMC Bioinformatics 10 (2009), p. 205.
- 38. J. Turner, *Almost all k-colorable graphs are easy to color*, Journal of Algorithms 9 (1988), pp. 63–82.
- 39. B. van Rietbergen, H. Weinans, R. Huiskes, and A. Odgaard, *A new method to determine trabecular bone elastic properties and loading using micromechanical finite-element models*, Journal of Biomechanics 28 (1995), pp. 69 81.
- 40. L. Wang, L. Zhou, J. Lu, and J. Yip, *An order-clique-based approach for mining maximal co-locations*, Information Sciences 179 (2009), pp. 3370–3382.

Appendix

Table 4. P1, P2, P3, P4 and P5 are the number of vertices pruned in steps Pruning 1, 2, 3, 4, and 5 of Algorithm 1. An asterisk (*) indicates that the algorithm did not terminate within 25,000 seconds for that instance. ω denotes the maximum clique size.

\overline{G}	ω	P1	P2	P3	P4	P5
cond-mat-2003	25	29,407	48,096	6,527	2,600	17,576
email-Enron	20	32,462	155,344	4,060	110,168	8,835,739
dictionary28	26	52,139	4,353	2,114	542	107
Fault_639	18	36	13,987,719	126	10,767,992	1,116
audikw_1	36	4,101	38,287,830	59,985	32,987,342	721,938
bone010	24	37,887	34,934,616	361,170	96,622,580	43,991,787
$af_shell10$	15	19	25,582,015	75	40,629,688	2,105
as-Skitter	67	1,656,570	6,880,534	981,810	26,809,527	737,899,486
roadNet-CA	4	1,487,640	1,079,025	370,206	320,118	4,302
kkt_power	11	1,166,311	4,510,661	401,129	1,067,824	1,978,595
rmat_er_1	3	780	1,047,599	915	118,461	8,722
rmat_er_2	3	2,019	2,094,751	2,351	235,037	23,908
rmat_er_3	3	4,349	4,189,290	4,960	468,086	50,741
rmat_er_4	3	9,032	8,378,261	10,271	933,750	106,200
rmat_er_5	3	18,155	16,756,493	20,622	1,865,415	212,838
rmat_sd1_1	6	39,281	1,004,660	23,898	151,838	542,245
$rmat_sd1_2$	6	90,010	2,004,059	56,665	284,577	1,399,314
rmat_sd1_3	6	176,583	4,013,151	106,543	483,436	2,677,437
$rmat_sd1_4$	6	369,818	8,023,358	214,981	889,165	5,566,602
rmat_sd1_5	6	777,052	16,025,729	455,473	1,679,109	12,168,698
rmat_sd2_1	26	110,951	853,116	88,424	1,067,824	614,813,037
rmat_sd2_2	35	232,352	1,645,086	195,427	81,886,879	1,044,068,886
rmat_sd2_3	39	470,302	3,257,233	405,856	45,841,352	1,343,563,239
$rmat_sd2_4$	43	*	*	*	*	*
rmat_sd2_5	N	*	*	*	*	*
hamming6-4	4	0	704	0	583	0
johnson8-4-4	14	0	1855	0	136,007	0
keller4	11	0	9435	0	8,834,190	0
c-fat200-5	58	0	8473	0	70449	0
brock200_2	12	0	9876	0	349,427	0

Table 5. Comparison of runtimes of algorithms [9] (*CP*), [28] (*cliquer*) and [21] (*MCQD+CS*) with that of our new exact algorithm (τ_{A1}) for DIMACS graphs. An asterisk (*) indicates that the algorithm did not terminate within 10,000 seconds for that instance. ω denotes the maximum clique size, ω_{A2} the maximum clique size found by our heuristic and τ_{A2} , its runtime.

				ı		_		
a	1171	l El			_	$ au_{MCQD}$		_
G	V	E	ω	$ au_{CP}$	$ au_{cliquer}$	+CS	$ au_{A1}$	ω_{A2} τ_{A2}
brock200_1	200	14,834	21	*	10.37	0.75	*	18 0.02
brock200_2	200	9,876	12	0.98	0.02	0.01	1.1	10 < 0.01
brock200_3	200	12,048	15	14.09	0.16	0.03	14.86	12 < 0.01
brock200_4	200	13,089	17	60.25	0.7	0.12	65.78	14 < 0.01
c-fat200-1	200	1,534	12	< 0.01	< 0.01	< 0.01	< 0.01	12 < 0.01
c-fat200-2	200	3,235	24	< 0.01	< 0.01	< 0.01	< 0.01	24 < 0.01
c-fat200-5	200	8,473	58	0.6	0.33	0.01	0.93	58 0.04
c-fat500-1	500	4,459	14	< 0.01	< 0.01	< 0.01	< 0.01	14 < 0.01
c-fat500-2	500	9,139	26	0.02	< 0.01	0.01	0.01	26 0.01
c-fat500-5	500	23,191	64	3.07	< 0.01	< 0.01	*	64 0.11
hamming6-2	64	1,824	32	0.68	< 0.01	< 0.01	0.33	32 < 0.01
hamming6-4	64	704	4	< 0.01	< 0.01	< 0.01	< 0.01	4 < 0.01
hamming8-2	256	31,616	128	*	0.01	0.01	*	128 0.67
hamming8-4	256	20,864	16	*	< 0.01	0.1	*	16 0.03
hamming10-2	1,024	518,656	512	*	0.31	-	*	512 95.24
johnson8-2-4	28	210	4	< 0.01	< 0.01	< 0.01	< 0.01	4 < 0.01
johnson8-4-4	70	1,855	14	0.19	< 0.01	< 0.01	0.23	14 < 0.01
johnson16-2-4	120	5,460	8	20.95	0.04	0.42	22.07	8 < 0.01
keller4	171	9,435	11	22.19	0.15	0.02	23.35	11 < 0.01
MANN_a9	45	918	16	1.73	< 0.01	< 0.01	2.5	16 < 0.01
MANN_a27	378	70,551	126	*	*	3.3	*	125 1.74
p_hat300-1	300	10,933	8	0.14	0.01	< 0.01	0.14	8 < 0.01
p_hat300-2	300	21,928	25	831.52	0.32	0.03	854.59	24 0.03
p_hat500-1	500	31,569	9	2.38	0.07	0.04	2.44	9 0.02
p_hat500-2	500	62,946	36	*	159.96	1.2	*	34 0.14
p_hat700-1	700	60,999	11	12.7	0.12	0.13	12.73	9 0.04
p_hat1000-1	1,000	122,253	10	97.39	1.33	0.41	98.48	10 0.11
san200_0.7_1	200	13,930	30	*	0.99	< 0.01	*	16 0.01