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On the maximum quasi-clique problem

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a b s t r a c t

Given a simple undirected graph $G = (V, E)$ and a constant $\gamma \in (0, 1)$, a subset of vertices is called a γ -quasi-clique or, simply, a γ -clique if it induces a subgraph with the edge density of at least γ . The maximum γ -clique problem consists in finding a γ -clique of largest cardinality in the graph. Despite numerous practical applications, this problem has not been rigorously studied from the mathematical perspective, and no exact solution methods have been proposed in the literature. This paper, for the first time, establishes some fundamental properties of the maximum γ -clique problem, including the NP-completeness of its decision version for any fixed γ satisfying $0 < \gamma < 1$, the quasi-heredity property, and analytical upper bounds on the size of a maximum γ -clique. Moreover, mathematical programming formulations of the problem are proposed and results of preliminary numerical experiments using a state-of-the-art optimization solver to find exact solutions are presented.

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1. Introduction

Networks or graphs, consisting of vertices (nodes, dots) and edges (links, arcs) connecting pairs of vertices, provide a convenient modeling tool for studying objects of diverse origins, including the Internet and the World Wide Web, natural ecosystems, cellular processes in biology, and phone call records in telecommunications, among other applications [\[21\]](#page-13-0). One of the common issues of interest to many such applications is finding large *clusters*, or ''tightly knit'' subsets of vertices. The ideal description of a cluster of similar elements is given by the concept of a *clique*, defined as a subset of vertices any two of which are connected by an edge. For example, in social networks, where the vertices correspond to ''actors'' and an edge indicates a relationship between two actors, a clique represents a group of people, any two of which have a certain kind of relationship (friendship, acquaintance, etc.) with each other [\[24\]](#page-13-1). In fact, some of the earliest work addressing the concept of cliques and methods of their detection was motivated by applications in sociometry [\[17](#page-12-0)[,16,](#page-12-1)[14\]](#page-12-2). Due to its numerous applications, the maximum clique problem is one of the most important NP-hard problems and it has been extensively studied in the literature. A detailed survey of results on the maximum clique problem and related references can be found in [\[8\]](#page-12-3).

While the clique model is, undoubtedly, a very reasonable formalization of a cluster, the requirement for every two vertices to be connected is rather restrictive for some applications, especially for those relying on experimental data. This motivated research on a variety of related concepts, some of which can be viewed as ''relaxations'' of the idea of clique. Not surprisingly, several such concepts first appeared in studying *cohesive subgroups* in social networks and were based

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on relaxing some of the desirable properties that a clique idealizes. The clique relaxation models originating from social network analysis include the notions of *k*-clique [\[16\]](#page-12-1), *k*-club [\[19\]](#page-13-2), and *k*-plex [\[23\]](#page-13-3); see also [\[6](#page-12-4)[,5\]](#page-12-5). Abello et al. [\[1,](#page-12-6)[2\]](#page-12-7) proposed a density-based relaxation called *quasi-clique*, which requires at least the fraction γ of all possible edges between vertices of a $γ$ -quasi-clique to be present. As a density-based relaxation, $γ$ -cliques provide a reasonable way for grouping objects that possess no inherent reason to display the structure of other clique relaxations. The previous literature related to the maximum γ -clique problem concentrated on heuristic detection of large quasi-cliques in various application scenarios. The goal of this paper is to start examining the maximum γ -clique problem from the mathematical perspective, including establishing the computational complexity of the problem for any fixed γ , exploring structural properties of γ -cliques, deriving analytical upper bounds, and developing mixed-integer programming (MIP) formulations.

The remainder of this paper is organized as follows. Section [2](#page-1-0) introduces the definitions and notations used throughout the paper. The NP-completeness of the decision version of the maximum γ -clique problem is proved in Section [3.](#page-1-1) Section [4](#page-2-0) defines the quasi-heredity property and establishes analytical bounds on the γ -clique number of a graph. Mathematical programming formulations are derived in Section [5](#page-5-0) and results of preliminary numerical experiments are reported in Section [6.](#page-6-0) Finally, Section [7](#page-11-0) concludes the paper.

2. Definitions, notations, and motivation

Let $G = (V, E)$ be a simple undirected graph with the set *V* of *n* vertices and the set *E* of *m* edges. For $u, v \in V, d_G(u, v)$ is the length of a shortest path between *u* and *v* in *G* and $d(G) = \max_{u,v \in V} d_G(u,v)$ is the diameter of *G*. Given $S \subseteq V$, $G[S] = (S, E \cap S \times S)$ denotes the subgraph induced by *S* on *G*. A graph $G = (V, E)$ is called *complete* if all its vertices are *pairwise adjacent, i.e. if* $∀i$, $j ∈ V$, $i ≠ j$, we have $(i, j) ∈ E$. A *clique C* is a subset of *V* such that the subgraph *G*[*C*] induced by *C* on *G* is complete. A clique is *maximal* if it is not a subset of a larger clique, and *maximum* if there is no larger clique in the graph. The maximum clique problem is to find a clique of maximum cardinality in *G*, which is called the *clique number* and is denoted by $\omega(G)$.

Given $G = (V, E)$ and fixed real γ satisfying $0 < \gamma < 1$, a subset of vertices 0 is called a γ -quasi-clique or, simply, a γ -clique if the edge density of the induced subgraph *G*[*Q*], which is given by the ratio of the number of edges in *G*[*Q*] to $\frac{|Q|}{2}$), is at least $\gamma.$ The maximum γ -clique problem asks for a γ -clique with the maximum possible number of vertices in *G*. We will denote the *γ*-clique number of a graph *G*, which is the cardinality of a largest γ -clique in *G*, by ω_{γ} *G*). Note that for $\gamma = 1$ the maximum γ -clique problem would become the classical maximum clique problem, while for $\gamma = 0$ the problem would be trivial. For a fixed $\gamma \in (0, 1)$ the problem has not been well studied. The earliest publication on the topic is attributed to Abello et al. [\[1\]](#page-12-6), who defined the concept of γ -quasi-clique and proposed greedy randomized adaptive search procedures (GRASP) for detecting large quasi-cliques in graphs representing telecommunications data.

Similar approaches were implemented in semi-external memory algorithms that handled massive graphs with hundreds of millions of vertices [\[2\]](#page-12-7). Several other papers, some of which use modified definitions of quasi-cliques, presented heuristic approaches to detecting large quasi-cliques in graphs arising in various applications [\[9,](#page-12-8)[7,](#page-12-9)[18](#page-12-10)[,22,](#page-13-4)[25](#page-13-5)[,15\]](#page-12-11). In summary, the previous work on the problem of interest concentrated mainly on heuristic detection of large quasi-cliques in graphs arising in a diverse set of applications. This paper provides a formal study of the computational complexity of the γ -clique problem, establishes analytical bounds on the γ -clique number and proposes mathematical programming formulations of the problem that can be used for finding provably optimal solutions.

3. Computational complexity

This section presents the computational complexity analysis for the maximum γ -clique problem for any fixed density γ between 0 and 1. To simplify the analysis, we first replace a real γ in the definition of a γ -clique with a rational $\frac{p}{q}$, where positive integers p and q ($p < q$) are given, resulting in the $\frac{p}{q}$ -clique model. Afterwards, the results obtained for $\frac{p}{q}$ -cliques will be extended to the general γ -clique case. Following the standard approach [\[13\]](#page-12-12), we define the recognition version of the problem, $\frac{p}{q}$ -Clique, as follows: Given a graph $G = (V, E)$ and positive integers p, q and k, does there exist a $\frac{p}{q}$ -clique of size at least *k* in *G*?

Proposition 1. The $\frac{p}{q}$ -CLIQUE problem is NP-complete for any positive integer constants p, q , $p < q$.

Proof. The proof is done by observing that $\frac{p}{q}$ -CLIQUE is, obviously, in the class NP and by reducing the classical CLIQUE problem to $\frac{p}{q}$ -Clique. Namely, for the given *k* and $\frac{p}{q}$, we will construct an auxiliary graph $G'=(V',E')$ and prove that *G* has a clique of size *k* if and only if *G* ∪ *G'* has a $\frac{p}{q}$ -clique of size $|V'| + k$.

The construction proceeds as follows. We build the set of vertices *V'* with $|V'| = 4(|V|^2 + k^2)q - k$ and construct edges to obtain a 2|*V*|-regular graph. It is easy to observe that one can always construct a graph with any specified even regularity, provided there are enough vertices. This can be done by, e.g., placing all the vertices of *V* ′ on a circle and connecting each vertex to its immediate |*V*| neighbors on each side in the circle. Next we randomly place edges so that we have $\frac{p}{q} \cdot {|\frac{|V'|+k}{2} - {k \choose 2}}$ edges between the $|V'|$ vertices. The value of $\frac{p}{q} \cdot {|\frac{|V'|+k}{2} - {k \choose 2}}$ is integer since $|V'|+k$ is a multiple of 2q. |V'| is sufficiently large to guarantee that the following inequalities hold:

$$
{|V'| \choose 2} \geq \frac{p}{q} {|V'| + k \choose 2} - {k \choose 2} \geq |V||V'|.
$$

The first inequality ensures that we can fit in the number of edges needed for a $\frac{p}{q}$ -clique of size $|V'| + k$ in $G \cup G'$, where k vertices would come from a clique in *G*. The second inequality allows one to build a 2|*V*|-regular graph on |*V*[']| vertices with no more edges than the desired value of $\frac{p}{q} {|\frac{|V'|+k}{2}} - {k \choose 2}.$

Consider the union $G \cup G'$ *of the two graphs. Then we can show that for any* $\frac{p}{q}$ *-clique <i>Q* with $|Q| > |V'|$ in $G \cup G'$ there exists a $\frac{p}{q}$ -clique *Q'* in *G* ∪ *G'* such that $|Q'| = |Q|$ and *V'* ⊂ *Q'*. Indeed, suppose that there is a $\frac{p}{q}$ -clique *Q* that has more than $|V'|$ vertices and does not include the entire V'. Define V_{in} to be the vertices from *G*' that are included in this $\frac{p}{q}$ -clique and *V*_{*out*} to be the ones missing. Then $|V_{out}| \leq |V|$, so a vertex from V_{out} cannot be connected to more than $|V| - 1$ vertices of *Vout*. Since every vertex in *G* ′ has degree at least 2|*V*|, each vertex in *^Vout* must be connected to at least |*V*| + 1 vertices in V_{in} . Therefore, any vertex from $Q \setminus V_{in}$ can be replaced with any vertex from V_{out} in Q with no reduction in the edge density of the subgraph induced by *Q*. Substituting arbitrary $|V_{out}|$ vertices from *Q* $\setminus V_{in}$ with V_{out} , we obtain a $\frac{p}{q}$ -clique *Q'* of the same size as *Q* that includes the entire *V* ′ .

To complete the proof, we will show that *G* has a clique of size *k* if and only if $G\cup G'$ has a $\frac{p}{q}$ -clique of size $|V'|+k$. Given a clique C of size k in G, combining G[C] with all of G' we have $|V'|+k$ vertices and $\frac{p}{q} \cdot { |V'| + k \choose 2} - {k \choose 2} + {k \choose 2} = \frac{p}{q} \cdot { |V'| + k \choose 2}$ edges, making this collection of vertices a $\frac{p}{q}$ -clique by definition. On the other hand, assuming that $G\cup G'$ has a $\frac{p}{q}$ -clique of $|V'| + k$ vertices, we know that there is $\frac{p}{q}$ -clique *Q'* of size $|V'| + k$ in *G* ∪ *G'* that contains all of the vertices from *G'* and hence precisely k of the vertices come from G. To see that the k vertices in Q \ V' form a clique, consider the density of G'. It is precisely $\frac{p}{q}\cdot\binom{|V'|+k}{2}-\binom{k}{2}$ by construction. If the *k* vertices from *G* don't contribute $\binom{k}{2}$ edges, then the set of $|V'|+k$ vertices forming Q cannot have density $\frac{p}{q}$. Thus the existence of a $\frac{p}{q}$ -clique of size $|V'| + k$ means the set of *k* vertices in the original graph induces a subgraph with $\binom{k}{2}$ edges and hence forms a clique. This establishes the NP-completeness of the *p q* -Clique problem.

Corollary 1. *For any given fixed real* $\gamma \in (0, 1)$ *, the* γ -CLIQUE *problem is NP-complete.*

Proof. First observe that instead of assuming that $\frac{p}{q}$ is a fixed value, we could allow $p = p(n)$ and $q = q(n)$ to be functions of *n* such that $0 < p(n) < q(n)$ and both $p(n)$ and $q(n)$ are $O(n^2)$. Clearly, any possible edge density for a graph on *n* vertices can be specified by $\frac{p(n)}{q(n)}$ with $p(n)$, $q(n) \leq n(n-1)/2$. The resulting $\frac{p(n)}{q(n)}$ -CLIQUE problem is also NP-complete, using the same proof we have given above. Based on this observation, it suffices to show that for any $\gamma \in (0, 1)$ there exist two functions $p(n)$, $q(n)$, of the order $O(n^2)$, such that $0 < p(n) < q(n)$ for any n, and the resulting $\frac{p(n)}{q(n)}$ -CLIQUE problem and γ -CLIQUE problem are equivalent.

Let γ be fixed. Define for any positive integer *s*

$$
\bar{p}(s) = \left\lceil \gamma \frac{s(s-1)}{2} \right\rceil, \qquad \bar{q}(s) = \frac{s(s-1)}{2}.
$$

Note that $\bar{p}(s)$ defines the minimum possible number of edges in the induced subgraph of any γ -clique of size *s*, so $\bar{p}(s)/\bar{q}(s) \geq \gamma$ and the actual edge density of any γ -clique of size *s* is at least $\bar{p}(s)/\bar{q}(s)$. Hence, any γ -clique of size *s* is also a $\frac{\bar{p}(s)}{\bar{q}(s)}$ -clique and vice versa. Next, for any positive integer *n* we define

$$
p(n) = \bar{p}(s^*), \qquad q(n) = \bar{q}(s^*), \quad \text{where } s^* = \arg\min_{1 \le s \le n} \frac{\bar{p}(s)}{\bar{q}(s)}.
$$

Then $0 < p(n) < q(n)$ for any *n* and $p(n)$, $q(n)$ are of order $O(n^2)$. Moreover, for any $s \le n$, any *s*-vertex subgraph $G_s = (V_s, E_s)$ of G is $\frac{p(n)}{q(n)}$ -clique if and only if it is a γ -clique, so $\frac{p(n)}{q(n)}$ -CLIQUE problem is equivalent to γ -CLIQUE problem.

4. Properties of γ**-cliques**

In this section we will discuss some properties of γ -cliques that may be useful in designing solution procedures for the maximum γ -clique problem. Unlike cliques, the γ -cliques fail to display a key property used in successful algorithms for the maximum clique problem: *heredity*. A property is called *hereditary* if, when it exists in a graph, it exists in all its induced subgraphs. It is easy to identify γ -cliques containing subsets of vertices that induce subgraphs with edge density less than γ . Because of this, even checking maximality by inclusion is a non-trivial task for quasi-cliques. However, γ -cliques do display a related property, which we will call *quasi-heredity*.

4.1. Quasi-heredity

If, given any graph $G = (V, E)$ satisfying a property P, there exists $v \in V$ such that $G - v := G[V \setminus \{v\}]$ also has property *P*, we call the property *P* a quasi-hereditary property and say that the property *P* displays *quasi-heredity* or *quasi-inheritance*.

Proposition 2. *The graph property of having edge density of at least* γ *displays quasi-inheritance. In other words, any* γ *-clique with s* > 1 *vertices is a strict superset of a* γ *-clique with s* $-$ 1 *vertices.*

Proof. Consider a γ -clique *Q* that induces a subgraph with *s* > 2 vertices and *e* edges (the statement is trivially true for $s = 2$). Then a smaller γ -clique of size $s - 1$ can always be formed by removing a vertex v with the lowest degree within Q. Since this vertex will have degree less than or equal to the average, which is given by 2*e*/*s*, the edge density of the subgraph induced by $Q \setminus \{v\}$ will be at least

$$
\frac{2e-4e/s}{(s-1)(s-2)} = \frac{2e}{s(s-1)},
$$

i.e., no less than that of *G*[*Q*], and hence $Q \setminus \{v\}$ is a γ -clique. \Box

The quasi-heredity property implies that, provided the vertices are placed in the right order, a maximum γ -clique can be found by starting with the first vertex in the list and sequentially adding the next vertex if the resulting subset of vertices is still a γ -clique. This gives us a hope that if we apply some "smart" vertex ordering rules, perhaps based on vertex degrees, there is a chance that we will be able to find large γ -cliques quickly (even though we cannot say how far their size will be from optimal). This observation suggests metaheuristic procedures such as GRASP [\[2\]](#page-12-7) as a natural choice for solving the problem of interest. The successful computational experience reported by Abello et al. [\[2\]](#page-12-7) provides practical evidence in support of this hypothesis.

4.2. Upper bounds

The proposed upper bound on the γ -clique number is a generalization of the classical Amin–Hakimi bound on the clique number [\[4\]](#page-12-13).

Proposition 3. *The* γ -clique number $\omega_{\gamma}(G)$ of a graph G with n vertices and m edges satisfies the following inequality:

$$
\omega_{\gamma}(G) \le \frac{\gamma + \sqrt{\gamma^2 + 8\gamma m}}{2\gamma}.
$$
 (1)

Moreover, if a graph G is connected then

$$
\omega_{\gamma}(G) \le \frac{\gamma + 2 + \sqrt{(\gamma + 2)^2 + 8(m - n)\gamma}}{2\gamma}.
$$
\n⁽²⁾

Proof. The first bound is obtained by solving the quadratic inequality

$$
\gamma \frac{\omega_{\gamma}(G)(\omega_{\gamma}(G)-1)}{2} \leq m.
$$

Assuming that the graph *G* is connected and has a γ -clique of size ω_{γ} (*G*), the following inequality must hold:

$$
\gamma \frac{\omega_{\gamma}(G)(\omega_{\gamma}(G)-1)}{2} + n - \omega_{\gamma}(G) \leq m.
$$

Solving this quadratic inequality for $\omega_{\nu}(G)$, we obtain the second bound. \square

For $\gamma = 1$ the second of the bounds becomes the Amin–Hakimi bound on the clique number, which is the only constanttime computable upper bound used in the comparison performed by Budinich [\[10\]](#page-12-14).

4.3. Relation between $\omega_{\nu}(G)$ *and* $\omega(G)$

Next we derive an inequality that will relate the γ -clique number to the clique number of *G*. We will need the following classical lower bound on the clique number that can be easily obtainedfrom the Motzkin–Straus [\[20\]](#page-13-6) formulation for the

The value of upper bound [\(5\)](#page-4-0) on γ -clique number $\omega_{\gamma}(G)$ ($\gamma = 0.95, 0.9, 0.85$) for graphs with known clique number $\omega(G) \in \{2, 3, ..., 10\}$. The bound does not depend on the size of *G* and only assumes that $\omega(G)$ is given by the value specified in the first column. Cases where the bound is not applicable (i.e., $\gamma\leq1-\frac{1}{\omega(G)}$) are marked with "-".

$\omega(G)$ $\frac{1}{\omega(G)}$		Bound (5) on $\omega_{\gamma}(G)$ for $\gamma = \cdots$				
		0.95	0.9	0.85		
\mathcal{L}	0.5	2.111	2.25	2.429		
3	0.667	3.35	3.86	4.64		
4	0.75	4.75	6	8.5		
5	0.8	6.33	9	17		
6	0.83	8.14	13.5	51		
7	0.86	10.23	21			
8	0.88	12.67	36			
9	0.89	15.55	81			
10	0.9	19				

maximum clique problem:

$$
\omega(G) \ge \frac{1}{1-\delta},\tag{3}
$$

where $\delta = 2m/n^2$.

Proposition 4. *The* γ -clique number $\omega_{\gamma}(G)$ and the clique number $\omega(G)$ of graph G satisfy the following inequalities:

$$
\frac{\omega(G)-1}{\omega(G)} \le \frac{\omega_{\gamma}(G)-1}{\omega_{\gamma}(G)} \le \frac{1}{\gamma} \frac{\omega(G)-1}{\omega(G)}.\tag{4}
$$

Proof. The first inequality is trivial due to the fact that $\omega(G) \leq \omega_{\gamma}(G)$. To prove the second inequality, consider a γ -clique *C* of largest size ω_{ν} (*G*) in *G*. Then, according to [\(3\),](#page-4-1) the size ω (*G*[*C*]) of the largest clique in the induced subgraph *G*[*C*] satisfies the inequalities

$$
\omega(G) \ge \omega(G[C]) \ge \frac{1}{1-\delta_C},
$$

where $\delta_C = 2m_C/n_C^2$, m_C is the number of edges in G[C], and $n_C = \omega_\gamma(G)$ is the number of vertices in G[C]. Since C is a γ -clique, we have

.

$$
\delta_C = \frac{2m_C}{n_C^2} = \frac{2m_C}{n_C(n_C-1)} \frac{n_C-1}{n_C} \ge \gamma \frac{n_C-1}{n_C}
$$

Therefore,

$$
\omega(G) \ge \frac{1}{1 - \gamma \frac{n_C - 1}{n_C}},
$$

which, taking into account that $n_C = \omega_\gamma(G)$, is equivalent to

$$
\frac{\omega_{\gamma}(G)-1}{\omega_{\gamma}(G)} \leq \frac{1}{\gamma} \frac{\omega(G)-1}{\omega(G)}.\quad \Box
$$

Corollary 2. If $\gamma > 1 - \frac{1}{\omega(G)}$ then

$$
\omega_{\gamma}(G) \le \frac{\omega(G)\gamma}{1 - \omega(G) + \omega(G)\gamma}.\tag{5}
$$

Proof. The result follows directly from the second inequality in [\(4\).](#page-4-2) \Box

Observe that bound [\(5\)](#page-4-0) on the *γ*-clique number ω _{*v*}(*G*) involves only one graph invariant, which is the clique number $\omega(G)$. Unlike more traditional bounds, such as [\(1\)](#page-3-0) or [\(2\),](#page-3-1) it does not explicitly depend on the number of vertices and edges in graph *G*, but instead assumes that the clique number of *G* is known. Such a bound can be especially useful for large sparse networks with a small clique number ω(*G*), assuming that ω(*G*) can be computed using effective scale-reduction procedures such as "peeling" used in [\[1\]](#page-12-6). As supporting evidence, [Table 1](#page-4-3) provides the value of bound [\(5\)](#page-4-0) with $\gamma = 0.95, 0.9, 0.85$ for

graphs with clique number in the range between 2 and 10. The first column of this table contains the value of the graph's clique number $\omega(G)$ (which is all one needs to know about *G* in order to compute bound [\(5\)](#page-4-0) on $\omega_{\nu}(G)$; the second column shows the value of threshold $1-\frac{1}{\omega(G)}$ needed to determine whether bound [\(5\)](#page-4-0) is applicable for given values of $\omega(G)$ and γ ; and the remaining three columns provide the value of bound [\(5\)](#page-4-0) for $\gamma=0.95, 0.9$, and 0.85, respectively. Since the bound is available only if $\gamma > 1-\frac{1}{\omega(G)}$, the cases when this condition is not met are marked with a dash in the table. As can be seen from the table, in some cases the bound appears to be extremely useful. For example, if one is given a very large, sparse graph *G* with $\omega(G) = 4$, it immediately follows from the bounds provided in the table that $\omega_{0.95}(G) = 4, 4 \le \omega_{0.9}(G) \le 6$, and $4 \leq \omega_{0.85}(G) \leq 8$.

5. MIP formulations of the maximum γ**-clique problem**

The lack of structure in γ -cliques as opposed to cliques and some other clique relaxations, such as *k*-plex [\[5\]](#page-12-5), makes this problem extremely difficult to solve to optimality. Indeed, the most successful combinatorial algorithms for the maximum clique and maximum *k*-plex problems rely on the heredity property of these structures, which is not an option in our case. Tight bounds and effective pruning strategies within a branch-and-bound framework are not easy to develop for the maximum γ -clique problem. This section develops mixed integer programming formulations for the maximum γ -clique problem.

We consider a graph $G = (V, E)$ with the set $V = \{1, \ldots, n\}$ of n vertices. We denote by $A = [a_{ij}]_{i,j=1}^n$ its adjacency matrix, which is an $n \times n$ matrix with a_{ii} equal to one if $(i, j) \in E$, and zero otherwise. We introduce *n* binary decision variables x_i , $i = 1, \ldots, n$, one for each vertex, such that the value x_i^* assigned to the variable x_i in the output optimal solution will indicate whether the corresponding vertex *i* is a part of the maximum γ -clique C^* computed. Namely, $i \in C^*$ if and only if $x_i^* = 1$. Then the maximum γ -clique problem can be formulated as follows:

$$
\omega_{\gamma}(G) = \max \sum_{i=1}^{n} x_i \tag{6}
$$

subject to

$$
\sum_{i=1}^{n} \sum_{j=i+1}^{n} a_{ij} x_i x_j \ge \gamma \sum_{i=1}^{n} \sum_{j=i+1}^{n} x_i x_j,
$$
\n(7)

$$
x_i \in \{0, 1\}, \quad i = 1, \dots, n. \tag{8}
$$

This problem has a linear objective, but its single constraint is quadratic. Next, we introduce new variables to make this problem linear. We define $w_{ij} = x_i x_j$. We need only $n(n-1)/2 - n$ new variables since $w_{ij} = w_{ji}$. The quadratic constraint $w_{ij} = x_i x_j$ with binary variables is equivalent to the following three linear constraints:

$$
w_{ij} \le x_i, \qquad w_{ij} \le x_j, \qquad w_{ij} \ge x_i + x_j - 1. \tag{9}
$$

Therefore, we can formulate our graph problem as a mixed integer linear optimization problem:

$$
\omega_{\gamma}(G) = \max \sum_{i=1}^{n} x_i,
$$
\n(10)

subject to

$$
\sum_{i=1}^n \sum_{j=i+1}^n (\gamma - a_{ij}) w_{ij} \leq 0, \tag{11}
$$

$$
w_{ij} \le x_i, \qquad w_{ij} \le x_j, \qquad w_{ij} \ge x_i + x_j - 1, \quad j > i = 1, \dots, n
$$
\n(12)

$$
w_{ij} \geq 0, \qquad x_i \in \{0, 1\}, \quad j > i = 1, \dots, n. \tag{13}
$$

This formulation contains $n(n-1)/2$ variables and $\frac{3}{2}n(n-1) + 1$ constraints.

Next we consider an alternative linearization. Recall that the original formulation $(6)-(8)$ had a single constraint that can be written as

$$
\sum_{i=1}^{n} x_i \left(\gamma x_i + \sum_{j=1}^{n} (a_{ij} - \gamma) x_j \right) \ge 0.
$$
 (14)

Let us define a new variable y_i for $i = 1, \ldots, n$ as follows:

 \overline{a}

$$
y_i = x_i \left(\gamma x_i + \sum_{j=1}^n (a_{ij} - \gamma) x_j \right). \tag{15}
$$

Let us use the following notations:

$$
u_i = (1 - \gamma) \sum_{j=1}^n a_{ij}; \qquad l_i = -\left(n - 1 - \sum_{j=1}^n a_{ij}\right) \gamma,
$$
\n(16)

where u_i is the sum of all the positive coefficients and l_i is the sum of all the negative coefficients for the variables in the expression in parenthesis of [\(15\).](#page-5-2) Since all variables are binary, the constants *uⁱ* and *lⁱ* satisfy the following inequalities:

$$
l_i \leq \gamma x_i + \sum_{j=1}^n (a_{ij} - \gamma) x_j \leq u_i, \quad i = 1, ..., n,
$$
 (17)

$$
l_i \leq y_i \leq u_i, \quad i = 1, \dots, n. \tag{18}
$$

Thus, the quadratic equality [\(15\)](#page-5-2) with binary variables is equivalent to the following four linear inequalities:

$$
y_i \le u_i x_i,\tag{19}
$$

$$
y_i \ge l_i x_i,\tag{20}
$$

$$
y_i \geq \gamma x_i + \sum_{j=1}^n (a_{ij} - \gamma) x_j - u_i (1 - x_i), \tag{21}
$$

$$
y_i \leq \gamma x_i + \sum_{j=1}^n (a_{ij} - \gamma) x_j - l_i (1 - x_i).
$$
 (22)

Therefore, the problem of finding a maximum γ -clique can be represented as the following mixed integer linear optimization problem with 2*n* variables, *n* of which are 0–1 variables and *n*-continuous, and 4*n* + 1 constraints:

$$
\omega_{\gamma}(G) = \max \sum_{i=1}^{n} x_i \tag{23}
$$

subject to

$$
\sum_{i=1}^{n} y_i \ge 0,\tag{24}
$$

$$
y_i \le u_i x_i, \qquad y_i \ge l_i x_i, \quad i = 1, \ldots, n,
$$
\n
$$
(25)
$$

$$
y_i \geq \gamma x_i + \sum_{j=1}^n (a_{ij} - \gamma) x_j - u_i (1 - x_i), \quad i = 1, ..., n,
$$
\n(26)

$$
y_i \leq \gamma x_i + \sum_{j=1}^n (a_{ij} - \gamma) x_j - l_i (1 - x_i), \quad i = 1, ..., n,
$$
\n(27)

$$
x_i \in \{0, 1\}; \qquad y_i \in \mathbb{R}, \quad i = 1, \dots, n. \tag{28}
$$

The proposed formulations allow one to use standard optimization solvers to find optimal γ -cliques in graphs that are not very large.

6. Results of numerical experiments

To provide a preliminary evaluation of the relative practical efficacy of the proposed mathematical programming formulations, sample numerical experiments have been conducted using a state-of-the-art commercial solver. All experiments were performed on a Dell Optiplex 980 PC with Intel Core i7 CPU 860 2.80 GHz processor, 8 GB RAM, running the 64-bit Windows 7 Professional operating system. The proposed formulations were used in conjunction with the FICO Xpress-IVE Version 1.21.02 solver on a number of instances.

The testbed used included three types of instances: uniform random graphs on 50 and 100 vertices, power-law random graphs on 100 vertices, and a set of standard test instances available in the public domain. Using random graph models provides a convenient and flexible framework for generating a wide range of instances allowing one to explore the capabilities and limitations of the proposed computational approaches. In addition to the commonly used uniform random graphs, we included a set of power-law random graphs in our testbed, which is motivated by a widely reported observation that many real-life complex networks appear to have power-law structure [\[12](#page-12-15)[,3,](#page-12-16)[21\]](#page-13-0). A uniformrandom graph *G*(*n*, *p*) has

Name	\boldsymbol{n}	\boldsymbol{p}	\boldsymbol{m}	$\omega_{\nu}(G)$ for $\gamma = \cdots$					
				$\mathbf{1}$	0.95	0.9	0.85	0.8	0.75
$u50-1$	50	0.2	215	$\overline{4}$	$\overline{4}$	5	5	6	7
$u50-2$	50	0.2	231	4	$\overline{4}$	5	5	$\,6$	$\,6$
$u50-3$	50	0.2	242	4	$\overline{4}$	5	5	6	6
$u50-4$	50	0.2	221	$\overline{4}$	$\overline{4}$	5	6	6	7
$u50-5$	50	0.2	253	$\overline{4}$	$\overline{4}$	5	6	6	$\overline{7}$
u50-6	50	0.3	355	5	5	6	$\overline{7}$	8	$9\,$
$u50-7$	50	0.3	379	5	5	5	6	7	8
$u50-8$	50	0.3	367	5	5	6	$\overline{7}$	8	9
u50-9	50	0.3	340	5	5	6	7	7	8
$u50-10$	50	0.3	354	5	5	6	$\overline{7}$	8	9
$u100-1$	100	0.05	244	3	3	3	3	$\overline{4}$	$\overline{4}$
u100-2	100	0.05	248	3	3	3	3	3	3
u100-3	100	0.05	217	4	$\overline{4}$	4	$\overline{4}$	5	5
u100-4	100	0.05	249	3	3	3	3	$\overline{4}$	$\overline{4}$
u100-5	100	0.05	280	3	3	3	3	$\overline{4}$	$\overline{4}$
u100-6	100	0.1	536	$\overline{4}$	$\overline{4}$	$\overline{4}$	$\overline{4}$	5	5
u100-7	100	0.1	485	4	4	4	$\overline{4}$	5	5
u100-8	100	0.1	500	4	4	5	5	$\,6$	6
u100-9	100	0.1	469	4	4	$\overline{4}$	$\overline{4}$	5	5
u100-10	100	0.1	490	$\overline{4}$	$\overline{4}$	4	$\overline{4}$	5	5
u100-11	100	0.15	737	$\overline{4}$	$\overline{4}$	5	6	6	7
u100-12	100	0.15	711	4	4	5	5	6	6
u100-13	100	0.15	741	$\overline{4}$	$\overline{4}$	5	5	6	7
u100-14	100	0.15	746	$\overline{4}$	4	5	6	6	7
u100-15	100	0.15	760	5	5	6	6	$\overline{7}$	8
u100-16	100	0.2	974	5	5	5	$\overline{7}$	$\overline{7}$	8
u100-17	100	0.2	934	5	5	6	$\overline{7}$	7	8
u100-18	100	0.2	977	5	5	6	6	7	8
u100-19	100	0.2	992	5	5	6	7	7	9
u100-20	100	0.2	1010	5	5	6	7	$\overline{7}$	8

Table 2 Description of the uniform random graphs used in experiments.

n vertices, where each pair of vertices is connected by an edge independently with the probability *p*, whereas in a powerlaw graph the probability that a vertex has degree *k* is proportional to *k*^{−β}. Generating test instances of uniform random graphs with given *n* and *p* is straightforward, whereas in the case of power-law graphs one can use the procedure described in [\[11\]](#page-12-17), which essentially assigns the probabilities p_{ij} for each pair of vertices (i, j) to be connected, using the extended random graph model for a general degree distribution and then adjusting that model so that the resulting graph follows the power-law degree distribution. As for standard test instances, we used some of the graphs from the Second and Tenth DIMACS Implementation Challenges (the corresponding links can be found at [http://dimacs.rutgers.edu/Challenges/\)](http://dimacs.rutgers.edu/Challenges/), as well as instances from Trick's graph coloring page [\(http://mat.gsia.cmu.edu/COLOR04/\)](http://mat.gsia.cmu.edu/COLOR04/).

[Tables 2–4](#page-7-0) present the description of the uniform random graphs, the power-law random graphs, and the standard test instances used, respectively. In [Table 2,](#page-7-0) the first column specifies the name of the graph, while the second and third columns labeled by "*n*" and "*p*" contain the number of vertices and probability used to generate the corresponding graph *G*(*n*, *p*), respectively. The next column ''*m*'' contains the actual number of edges in the corresponding graph. The remaining columns show the computed γ -clique number $\omega_{\gamma}(G)$ for $\gamma = 1, 0.95, 0.9, 0.85, 0.8,$ and 0.75. The only difference in notations used in [Table 3](#page-8-0) compared to [Table 2](#page-7-0) is in the third column, where the parameter β needed to generate a power-law random graph is used instead of p. Finally, the column labeled by " ρ " in [Table 4](#page-8-1) contains the graph's edge density, $\rho = \frac{2m}{n(n-1)}$. The first six graphs in the standard instances set listed in [Table 4](#page-8-1) are from DIMACS Challenges (with the first graph being from the Second DIMACS Implementation Challenge and the other five from the Tenth DIMACS Implementation Challenge), and the remaining instances are from the graph coloring collection. The selection of this subset of well-known graphs, available in the public domain, which excludes larger-scale instances, was driven by limitations of the proposed solution approaches and can be justified by computational intractability of the maximum quasi-clique problem.

The running times for the two proposed formulations applied to the above described uniform random graphs, power-law random graphs, and standard test instances are compared in [Tables 5–7,](#page-9-0) respectively. The first column of these tables, again, contains the graph name. The remaining eight columns are subdivided into four pairs corresponding to four reported values of γ ; $\gamma = 1$, 0.95, 0.85, and 0.75, respectively. In each of the four pairs of columns, the first column, marked with "F1", shows the running time for formulation [\(10\)–\(13\),](#page-5-3) and the second column, "F2", reports the running time for formulation [\(23\)–\(28\).](#page-6-1) All running times are reported in seconds. If the MIP gap did not show much improvement after 50,000 s, the corresponding

Description of standard test instances used in experiments.

run was terminated with ">50,000" reported in the respective table entry. One can observe that, in most cases, the running times for both formulations grow significantly with the increase of graph density and the decrease in γ value. While the second formulation consistently outperforms the first one for higher values of γ on the considered uniform random graphs, the first formulation takes over when $\gamma~\leq~0.85$ and the graph's edge density is at least 0.15. The difference becomes dramatic on the last 10 graphs in [Table 5](#page-9-0) and the last 5 instances in [Table 6,](#page-9-1) for which the second formulation requires

Comparison of running times for the experiments with power-law random graphs.

over 50,000 s in multiple cases, while the first one often finds the solution in much shorter time spans and never takes more than 40,000 s. Similar conclusions can be made with respect to the results reported for standard instances. Running times become prohibitively high with an increase in edge density for lower values of γ , especially for the second formulation. In the most extreme example, the execution of the second formulation for "johnson8-2-4" with $\gamma = 0.75$ has not terminated

Graph	Running times, in seconds, for $\gamma = \cdots$							
	$\mathbf{1}$		0.95		0.85			
	F ₁	F ₂	F1	F ₂	F ₁	F ₂	F1	F ₂
Johnson8-2-4	0.1	0.0	0.7	1.1	1.7	752.7	20.0	> 50,000
Karate	0.1	0.0	0.6	0.6	0.7	0.5	0.9	0.8
Dolphins	0.4	0.3	5.1	1.6	5.2	3.2	5.3	7.8
Polbooks	2.1	0.3	146.2	10.1	99.8	46.4	749.5	1160.9
Adjnoun	2.5	0.7	132.2	9.7	147.0	46.9	462.0	706.4
Football	2.2	0.4	299.9	12.2	268.1	108.2	2077.0	22,392.4
Games 120	2.0	0.5	372.4	16.4	237.8	414.5	2968.8	> 50,000
Myciel3	0.0	0.1	0.1	0.2	0.1	0.2	0.1	0.2
Myciel4	0.1	0.1	0.3	1.0	0.3	0.5	0.4	1.0
Myciel5	0.5	0.3	2.7	1.5	3.7	4.4	7.8	84.0
Myciel ₆	3.8	1.2	65.7	16.3	409.1	13,530.1	2184.9	> 50,000
Queen5_5	0.1	0.0	0.4	0.7	0.8	2.4	1.3	602.9
Queen6_6	0.5	0.1	1.4	2.6	3.7	33.3	20.4	15,838.2
Queen7_7	0.8	0.2	4.3	6.0	27.0	4840.6	359.8	> 50,000
1-FullIns_3	0.1	0.1	0.6	0.6	0.7	0.7	0.8	0.9
2-FullIns_3	0.3	0.1	3.0	1.2	3.5	3.1	4.4	9.9
3-FullIns_3	0.7	0.1	10.1	4.0	15.0	22.3	27.9	163.9
4-FullIns_3	1.3	0.1	224.2	11.5	203.3	136.7	1502.2	4819.0
5-FullIns_3	3.0	1.1	1115.8	31.3	791.8	2013.4	6829.2	> 50,000
1-FullIns_4	1.3	0.3	65.0	10.5	230.8	447.9	1100.5	> 50,000
1-Insertions_4	0.6	0.2	6.6	2.5	6.8	4.9	9.9	25.6
2-Insertions_3	0.1	0.0	1.1	0.9	1.0	0.8	1.2	0.6
3-Insertions_3	0.2	0.0	2.9	1.4	3.2	2.0	3.5	2.2
4-Insertions_3	0.6	0.1	8.2	3.0	7.8	4.2	10.1	10.0
Mug88_1	0.7	0.2	9.8	4.7	78.1	6.0	77.6	9.3
Mug88_25	0.7	0.2	7.8	5.0	72.8	5.9	73.6	10.1
Mug100_1	1.0	0.2	15.1	6.8	143.9	5.2	143.3	15.4
Mug100_25	2.1	0.2	14.3	3.8	146.2	4.8	141.7	13.2
Huck	0.7	0.2	8.7	3.6	11.9	13.0	23.4	527.0
Jean	0.7	0.1	9.0	3.5	13.0	8.2	18.3	25.5
David	0.8	0.1	49.3	6.6	45.7	83.6	281.2	957.5
Anna	2.2	0.7	280.1	22.8	418.6	1142.0	652.9	4684.3

Table 7 Comparison of running times for the experiments with standard test instances.

after 50,000 s. The graph in question has only 28 vertices, but its edge density is over 0.5. The poor performance of the considered approaches on dense graphs is the main reason why ''johnson8-2-4'' was the only instance from the Second DIMACS Implementation Challenge included in our testbed. The other instances from this collection appeared to be too challenging for the studied approaches to be able to compute $\omega_{\nu}(G)$ values for every γ in the considered range within the 50,000 s time limit or have over 0.9 edge density and thus are trivial for $\gamma < 0.9$. The largest nontrivial standard instance from the testbed that we were able to solve to optimality for all considered γ values was "5-FullIns_3" from the graph coloring collection. This graph consists of 154 vertices and 792 edges.

To provide a deeper insight into the performance of the two formulations, [Tables 8](#page-11-1) and [9](#page-12-18) present a comparison of upper bounds on $\omega_{\gamma}(G)$ for selected random graphs and standard instances, respectively. The first bound is based on analytical expression (1) (if the graph is not connected; such graphs are marked with *) or (2) (for connected graphs). The other two bounds are given by the optimal objective function value of LP relaxations for the first formulation (LPRF1), and the second formulation (LPRF2). Solving times for the LP relaxations are given in seconds. For random graphs, one representative problem instance from each subtype included in the testbed is used for the comparison. All uniform random graphs generated for the experiments were verified to be connected, therefore, upper bound (2) applies. On the other hand, none of the power-law random graphs in the testbed were connected, therefore, bound (1) was used for the corresponding two instances included in [Table 8.](#page-11-1) The standard instances in [Table 9](#page-12-18) were selected to illustrate the fact that none of the bounds is dominated by another. Only two of all the considered standard instances are disconnected, and both of them are included in the table. One can observe that in most cases both LP bounds are of rather poor quality and could be improved by adding the constraints corresponding to the proposed analytical bounds. However, adding such constraints results in even higher running times, as finding high-quality feasible solutions becomes more challenging for the MIP solver. The LP bounds obtained from the MIP formulations are comparable, with the second formulation being slightly tighter in most cases. Moreover, the LP relaxation of the second formulation requires less time to compute. Surprisingly, the first formulation still comprehensively outperforms the second one on several instances, as reported in [Tables 5–7.](#page-9-0) This is due to the fact that typically the number of branch-and-bound nodes explored by the solver for the first formulation is significantly lower than

Comparison of upper bounds for selected random graphs. For analytical bound, (1) is used for disconnected graphs (marked with [∗]), and (2) is used for connected graphs.

Graph	γ	Analytical bound	LPRF1		LPRF ₂		
			Bound	Time	Bound	Time	
$u50-1$	0.75	22.8895	26.0652	0.187	25.9913	0.032	
	0.85	21.4513	25.5849	0.187	25.5126	0.032	
	0.95	20.2550	25.1768	0.218	25.1501	0.031	
	$\mathbf{1}$	19.7277	25.0000	0.078	25.0000	0.031	
u50-6	0.75	30.4112	27.056	0.234	26.9876	0.032	
	0.85	28.5178	26.1010	0.202	26.0082	0.032	
	0.95	26.9399	25.3336	0.202	25.2911	0.032	
	$\mathbf{1}$	26.2437	25.0000	0.093	25.0000	0.031	
$u100-1$	0.75	21.5148	50.4621	0.951	50.4469	0.094	
	0.85	20.1598	50.2447	0.999	50.2352	0.093	
	0.95	19.0332	50.073	0.983	50.0698	0.093	
	$\mathbf{1}$	18.5367	50.0000	0.328	50.0000	0.093	
u100-6	0.75	35.9805	51.0966	1.123	51.0581	0.093	
	0.85	33,7497	50.5881	1.186	50.5538	0.109	
	0.95	31.8892	50.1763	1.373	50.1637	0.109	
	$\mathbf{1}$	31.0677	50.0000	0.296	50.0000	0.110	
u100-11	0.75	43.0890	51.6616	1.529	51.5565	0.109	
	0.85	40.4274	50.9068	1.716	50.8102	0.110	
	0.95	38.2059	50.2771	2.169	50.2385	0.093	
	$\mathbf{1}$	37.2246	50.0000	0.312	50.0000	0.093	
u100-16	0.75	50.1451	52.2528	2.199	52.1858	0.110	
	0.85	47.0558	51.2018	1.451	51.1319	0.109	
	0.95	44.4759	50.3610	1.544	50.3319	0.125	
	$\mathbf{1}$	43.336	50.0000	0.312	50.0000	0.093	
pl100-1*	0.75	29.3487	50.6982	2.277	50.6889	0.109	
	0.85	27.5992	50.3720	2.463	50.3572	0.110	
	0.95	26.1338	50.1110	2.292	50.1048	0.109	
	$\mathbf{1}$	25.4850	50.0000	0.296	50.0000	0.094	
pl100-11*	0.75	51.4665	53.2654	4.054	53.7225	0.140	
	0.85	48.3750	51,7716	3.660	51.8166	0.100	
	0.95	45.7855	50.5436	3.809	50.5103	0.100	
	1	44.6390	50.0000	0.310	50.0000	0.100	

for the second formulation. For example, for graph u50-1 with $\gamma = 0.75$ the first formulation terminates at node 541, while the second formulation terminates at node 17,459. It should be noted that in the reported preliminary experiments we used default solver settings. Perhaps more advanced branch-and-bound strategies, tailored specifically for the maximum quasi-clique problem, may lead to significant speedups.

7. Conclusion

This paper is the first attempt to establish rigorous mathematical foundations for the maximum γ -clique problem that finds numerous practical applications. We show that the decision version of the problem is NP-complete, develop analytical bounds on the γ -clique number of a graph, and provide mixed-integer programming formulations for the problem of interest. In addition, we report the results of a preliminary computational study employing the proposed formulations in conjunction with a modern commercial MIP solver. The lack of well-defined structure in γ -cliques makes the problem extremely challenging for exact solution methods. The results of numerical experiments underline the necessity of developing more advanced techniques in order to be able to solve larger-scale instances to optimality. We hope that the analytical bounds and MIP formulations proposed in this paper will motivate future research on exact algorithms for the maximum quasi-clique problem.

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Comparison of upper bounds for selected standard instances. For analytical bound, (1) is used for disconnected graphs (marked with [∗]), and (2) is used for connected graphs.

Graph	γ	Analytical bound	LPRF1		LPRF2	
			Bound	Time	Bound	Time
Johnson8-2-4	0.75	23.9398	17.6842	0.060	17.6842	0.020
	0.85	22.4381	15.7355	0.055	15.7355	0.015
	0.95	21.1885	14,4762	0.055	14,4762	0.015
	$\mathbf{1}$	20.6377	14	0.035	14	0.015
Football	0.75	38.3212	58.5086	7.755	58.5079	0.125
	0.85	35.9485	58.0312	8.400	58.0291	0.125
	0.95	33.9692	57.6582	8.295	57.6568	0.125
	$\mathbf{1}$	33.0951	57.5	0.365	57.5	0.115
Myciel4	0.75	13.2946	12.5244	0.030	12.3947	0.020
	0.85	12.4353	12.0637	0.030	11.9553	0.015
	0.95	11.7243	11.6699	0.030	11.6317	0.015
	$\mathbf{1}$	11.4121	11.5	0.025	11.5	0.015
Queen _{7_7}	0.75	35.6272	27.7114	0.230	27.718	0.035
	0.85	33.4179	26.1819	0.170	26.1008	0.035
	0.95	31.5753	25.0204	0.185	24.9557	0.035
	$\mathbf{1}$	30.7617	24.5	0.075	24.5	0.03
5-Fullins_3	0.75	43.1213	78.056	32.585	77.9992	0.215
	0.85	40.4577	77.557	39.365	77.5234	0.255
	0.95	38.2346	77.1656	34.585	77.1548	0.220
	$\mathbf{1}$	37.2526	77	0.810	77	0.190
Mug100_1	0.75	15.2259	50.2922	0.550	50.2913	0.090
	0.85	14.2504	50.1544	0.590	50.1538	0.095
	0.95	13.442	50.046	0.575	50.0458	0.090
	$\mathbf{1}$	13.0866	50	0.280	50	0.085
Huck*	0.75	28.8358	38.3131	0.605	38.3104	0.060
	0.85	27.1174	37.8462	0.740	37.6622	0.055
	0.95	25.6781	37.3961	1.475	37.1905	0.055
	$\mathbf{1}$	25.0408	37	0.160	37	0.050
Jean*	0.75	26.5304	40.8676	0.800	40.7582	0.070
	0.85	24.9519	40.516	0.810	40.3911	0.065
	0.95	23.6298	40.1554	1.325	40.1143	0.070
	1	23.0444	40	0.180	40	0.055

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