On Maximum 2-Clubs

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Abstract -

We consider the Maximum 2-Club problem where one is given as input an undirected graph G = (V, E) and seeks a subset of vertices S of maximum size such that any pair of vertices in S is connected by a path of length at most 2 in the graph induced by S. This problem is a natural relaxation of the famous Maximum Clique problem where any pair of vertices must be connected by an edge. Maximum 2-Club has been well-studied and is known to be NP-complete even on split graphs. It can be solved exactly in $O^*(1.62^n)$ time, where n denotes the number of vertices of the input graph, while being polynomial-time solvable on several graph classes. Parameterized algorithms for structural parameters have also been considered, leading in particular to an algorithm with a double-exponential dependence in the parameter treewidth. Such an algorithm is actually the best one known for the larger parameter vertex cover size up to a constant in the exponent. We provide new results in both directions. We first prove that the double-exponential dependence for parameter vertex cover size is unavoidable under the Exponential Time Hypothesis (ETH). This answers a question left open by Hartung, Komusiewicz, Nichterlein and Suchỳ [14]. Our result also implies that the problem cannot be solved in time sub-exponential in n even for split graphs. We then provide an exact algorithm for the problem restricted to chordal graphs, running in $O^*(1.1996^n)$ time, by reducing Maximum 2-Club on this class to Maximum Independent Set on arbitrary graphs with the same number of vertices. The same reduction shows that we can enumerate all maximum (and inclusion-wise maximal) 2-clubs of a chordal graph in $O^*(3^{\frac{n}{3}}) = O^*(1.4423^n)$ time. We conclude by providing a construction of split graphs with $\Omega(3^{\frac{n}{3}}/\text{poly}(n))$ maximum 2-clubs, for some polynomial poly showing that the bound for enumeration is essentially tight.

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1 Introduction

Finding large sets of densely connected subgraphs in a given graph has been a challenging task for decades, with applications ranging from social networks to biological networks (see, e.g., [10]). To that extent, one of the most famous problems is MAXIMUM CLIQUE where one seeks the largest subset of vertices pairwise connected by an edge. MAXIMUM CLIQUE is one of the earliest NP-hard problems [9] and, from a parameterized complexity viewpoint, one of the most classical examples of a W[1]-hard problem (see e.g. [7]). However, the problem

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becomes tractable on many well-studied graph classes such as perfect graphs, circle graphs or unit disk graphs, see e.g. [5, 12, 22]. In particular, it becomes easy on many classes of *sparse graphs*, that often contain polynomially many maximal cliques [19, 21, 25]. Nonetheless, such graphs generally do not contain large cliques which is one of the reasons for considering relaxations of the notion of clique.

Many properties of being a clique can be used to define such relaxations. For instance, considering the degree leads to the notion of p-core where every vertex in the set S must have degree at least p in the subgraph induced by S. A closely related notion is that of a p-plex, where each vertex of S is required to have degree at least |S|-p. When considering density, namely the fraction of present edges with respect to the total possible number, the natural relaxation is that of a δ -quasi-clique where the density must be at least δ (note that $\delta=1$ amounts to a clique while $\delta=0$ can be any subset of the vertices). We refer the reader to the paper of Komusiewicz [16] and the thesis of Castillon [3] for a more comprehensive description of such relaxations.

In this work, we consider relaxations that are connected to the diameter of the sought subset. The diameter of a graph is the length of its longest shortest path. Two relaxations can be naturally defined with this property: for a given integer s, one may either seek for the largest set S where the distance between any two vertices is at most s in G or require that this property holds in the subgraph of G induced by S. The former case leads to the notion of s-clique while the latter is called s-club. We focus on the notion of s-club and especially the case s=2 which corresponds to the notion closest to being a clique. Formally, we consider the following problem.

Maximum 2-club

Input: A simple, undirected graph G = (V, E)

Output: Does there exist a 2-club of size at least ℓ in G?

Related work

This problem is well-studied from both the structural and algorithmic viewpoints. As for the MAXIMUM CLIQUE problem, the largest 2-club can be found in polynomial time in many graph classes such as bipartite graphs, trees and interval graphs [23]. Similarly, Golovach et al. [11] prove the polynomial-time solvability of the s-club problem on chordal bipartite, strongly chordal and distance-hereditary graphs. In sharp contrast, MAXIMUM s-Club is NP-complete on graphs of diameter s+1 for all $s \ge 1$. The MAXIMUM 2-CLUB problem is NP-complete even on split graphs and, thus, also on chordal graphs [1]. Moreover, the complexity of s-club is well-understood in a large class of graphs, called weakly chordal graphs: it is polynomial-time solvable for odd s and NP-hard for even s [11]. The MAXIMUM 2-CLUB problem has been well-studied from both parameterized complexity and exact algorithms perspectives. It is possible to design a branching algorithm with running-time $O(2^{n-\ell} \cdot poly(n))$ for the dual parameter $n-\ell$ [24]. It is proved in [13] that, unless the Strong Exponential Time Hypothesis fails, such an algorithm cannot be improved to $O((2-\epsilon)^{n-\ell} \cdot nm)$ for any $\epsilon > 0$. Chang et al. show that the s-club problem can be solved in $O(1.62^n)$ -time [4]. Hartung, Komusiewicz and Nichterlein [13] proved that a maximum 2-club can be found in time $2^{O(2^{tw})} \cdot n^2$ where tw denotes the treewidth of the input graph. They also presented an algorithm with the same complexity (up to a constant in the exponent) regarding the larger parameter vertex cover size. Then in [14], Hartung, Komusiewicz, Nichterlein and Suchý

provide double-exponential FPT algorithms for two other parameters: the vertex deletion distance to cluster graphs (i.e. graphs in which every connected component induces a clique), and for vertex deletion to cographs (graphs that do not admit a path on four vertices as an induced subgraph).

Our results

We investigate the MAXIMUM 2-CLUB problem from both algorithmic and structural aspects. We first consider structural parameterizations of the problem. We provide evidence that the algorithm by Hartung, Komusiewicz and Nichterlein [13], whose dependency on the vertex cover size vc(G) is $2^{O(2^{vc})}$ is essentially the best one can hope for assuming the Exponential Time Hypothesis holds. Our result actually holds even for split graphs (the vertex set of a split graph being partitionable into a maximal clique and an independent set, the size of a vertex cover is at most that of a maximum clique which implies the claimed result) and also implies a sub-exponential time lower bound on such graphs.

▶ **Theorem 1.** If there exists an algorithm which, given as input a split graph G = (V, E), computes the maximum size of a 2-club $S \subseteq V$ of G and runs in time $2^{2^{o(\omega(G))}}2^{o(|V|)}$, where $\omega(G)$ is the maximum size of a clique of G, then the ETH is false.

As a consequence, the double-exponential algorithms parameterized by treewidth [13], by vertex deletion distance to cluster graphs, and by vertex deletion to cographs [14] are essentially tight, since the vertex cover size is greater than or equal to all other parameters.

We then turn our attention to exact algorithms and provide an improved exact algorithm for this problem on chordal graphs. Our algorithm relies on the simple observation that any 2-club that is not a clique must intersect a minimal separator. Then, by a careful analysis of the remaining possibilities, we observe that the problem can be reduced to that of finding a maximum-sized independent set in an auxiliary graph with the same number of vertices. Since all minimal separators of a chordal graph can be enumerated in linear time (see e.g. [17]) and since a maximum independent set in n-vertex graphs can be found in time $O^*(1.1996^n)$ [26], we obtain the following.

▶ **Theorem 2.** The maximum 2-club of a chordal graph G can be found in time $O^*(1.1996^n)$.

This reduction to MAXIMUM INDEPENDENT SET can also be used to enumerate all maximum (or inclusion-wise maximal) 2-clubs of a chordal graph in time $O^*(3^{\frac{n}{3}})$, using the enumeration algorithm of maximal independent sets of [18], with the same running time.

▶ **Theorem 3.** Chordal graphs have $O^*(3^{\frac{n}{3}})$ maximal 2-clubs, enumerable within the same running time.

Note that n-vertex graphs can have up to $3^{\frac{n}{3}}$ maximum (or inclusion-wise maximal) independent sets as shown by a disjoint union of n/3 triangles, and this upper bound is tight [18]. We prove that a similar situation occurs when counting/enumerating the maximum (or inclusion-wise maximal) 2-clubs of chordal graphs, or even split graphs, by showing that there exist split graphs having $\Omega^*(3^{\frac{n}{3}})$ maximum (or inclusion-wise maximal) 2-clubs. As a byproduct, the bound of Theorem 3 is tight.

▶ Theorem 4. For any $n \in \mathbb{N}$, there exists a split graph G of n vertices that contains $\Omega(3^{\frac{n}{3}}/\operatorname{poly}(n))$ distinct maximum (and inclusion-wise maximal) 2-clubs, for some fixed polynomial poly.

2 Preliminaries

We consider simple, undirected graphs G = (V, E) where V denotes the vertex set of G and E its edge set. We sometimes use V(G) and E(G) to clarify the context. Given a vertex v of G, we let N(v) denote the open neighborhood of v, that is $N(v) = \{u \in V : uv \in E\}$. The closed neighborhood of v, denoted N[v] is defined as $N(v) \cup \{v\}$. Given a subset of vertices S of G, we let $N(S) = \bigcup_{s \in S} N(s) \setminus S$ denote the open neighborhood of S. The closed neighborhood of S is similarly defined as $N[S] = N(S) \cup S$. We sometimes add a reference to G in the notation, namely $N_G(v)$ and $N_G[v]$ to clarify the context (and similarly for subsets S). The subgraph induced by S is defined as $G[S] = (S, E_S)$ where $E_S = \{uv \in E : (u, v) \in S^2\}$. For simplicity let G - S denote the graph $G[V \setminus S]$.

A path $P=(x_1,\ldots,x_p)$ is a sequence of distinct vertices such that every pair of successive vertices are adjacent. If moreover $x_1x_p\in E$ then (x_1,\ldots,x_p) is a cycle. The length of a path is its number of vertices, minus one. Given two vertices u and v of G the length of a shortest path between u and v in G is denoted as $dist_G(u,v)$. For the sake of simplicity, for a given subset of vertices S of V(G) we use $dist_S(u,v)$ to denote $dist_{G[S]}(u,v)$. The diameter of a graph G is the maximum length of any of its shortest paths.

Throughout the paper we will consider several special subsets of vertices and graph classes. A clique is a set of pairwise adjacent vertices while an independent set is a set of pairwise non-adjacent vertices. Given a graph G=(V,E) with |V|=n vertices and an integer $1\leqslant s\leqslant n$, a subset $S\subseteq V$ is an s-club if the diameter of G[S] is at most s. In all cases the classical associated problems ask for a set of maximum cardinality with the desired property. A graph is a split graph if it can be partitioned into a clique and an independent set. A graph is chordal if every cycle with at least 4 vertices has a chord, that is, an edge between two non-consecutive vertices of the cycle.

A vertex cover of G is a set of vertices that intersects all the edges of the graph. The vertex cover size of graph G, denoted vc(G), is the minimum size of a vertex cover (sometimes, when it is clear from the context, we simply speak of the "vertex cover of G" to refer to the vertex cover size). The maximum size of a clique is denoted $\omega(G)$. In a split graph G the two parameters are strongly related, since $\omega(G) - 1 \le vc(G) \le \omega(G)$.

In a graph G = (V, E), a subset $S \subseteq V$ is a *separator* for two vertices u and v if removing S from G separates u and v in two distinct connected components. The set S is a *minimal separator* for u and v if moreover no proper subset of S separates u and v. We also say that S is a (u, v)-separator, respectively a (u, v)-minimal separator.

▶ **Lemma 5** (folklore). Let S be a (u,v)-minimal separator and let C_u (res. C_v) be the connected component of G-S containing u (resp. v). Then $N_G(C_u)=N_G(C_v)=S$.

The following observation is a well-known fact about chordal graphs. Here, we simply call *minimal separator* of G a vertex set S that is a (u, v)-minimal separator for some pair (u, v) of vertices.

▶ **Observation 6** ([6]). A graph G is chordal if and only if each minimal separator of G is a clique.

The Exponential Time Hypothesis (ETH) formulated by Impagliazzo and Paturi [15] conjectures that the 3-SAT problem cannot be solved in sub-exponential time. The Strong Exponential Time Hypothesis (SETH) assumes that, for all $\delta < 1$, there exists a k such that k-SAT cannot be solved in $O(2^{\delta n})$ time [2]. In other words, this hypothesis implies that SAT cannot be solved in $O(2^{\delta n})$ time for any $\delta < 1$.

By standard reduction from 3-SAT to MAXIMUM INDEPENDENT SET (see also Corollary 11.10 in the book of Fomin and Kratsch [8]), we have that the latter problem cannot be solved in time $2^{o(n+m)}$ unless ETH fails.

▶ Theorem 7. Unless ETH fails, there is no $2^{o(n+m)}$ algorithm for MAXIMUM INDEPENDENT SET.

Finally, we use the O^* notation to indicate that polynomial factors are omitted from the expression. That is, we write $O^*(f(n))$ whenever the complexity is $O(f(n) \cdot poly(n))$. We also use the $\Omega^*(f(n))$ notation to refer to functions $\Omega(f(n)/\operatorname{poly}(n)))$ for some polynomial poly.

3 Lower Bound for Maximum 2-club parameterized by vertex cover

Recall that $\omega(G)$ denotes the maximum clique size of G which, if G is a split graph, can be computed in polynomial time. We show that computing the largest 2-club (i.e., solving problem MAXIMUM 2-CLUB) has a double-exponential dependence parameterized by the clique size of a split graph, assuming ETH. Because in a split graph the maximum clique size is almost equal to the minimum vertex cover $(\omega(G) - 1 \le \text{vc}(G) \le \omega(G))$, this implies that the problem has at least double-exponential parameter dependence when parameterized by vertex cover. Furthermore, because the theorem is based on a reduction from MAXIMUM INDEPENDENT SET with only a linear blow-up in size, we can also conclude by Theorem 7 that, even for split graphs, the problem cannot be solved in time sub-exponential in the order of the input graph.

▶ **Theorem 1.** If there exists an algorithm which, given as input a split graph G = (V, E), computes the maximum size of a 2-club $S \subseteq V$ of G and runs in time $2^{2^{o(\omega(G))}}2^{o(|V|)}$, where $\omega(G)$ is the maximum size of a clique of G, then the ETH is false.

Proof. We present a reduction from MAXIMUM INDEPENDENT SET. Suppose we are given a graph G = (V, E) on n vertices and m edges and are asked if G has an independent set of size at least s. We will construct a split graph G' and a target size s' with the following properties:

- 1. G' has a 2-club of size at least s' (that is, a set of vertices S with $|S| \geq s'$ and the diameter of G'[S] being at most 2) if and only if G has an independent set of size s.
- 2. G' is split and its maximum clique size is $\omega(G') = O(\log n)$.
- 3. |V(G')| = O(n+m) and the construction can be carried out in polynomial time.

Let us first observe that if we achieve the above, we obtain the theorem. Indeed, we can decide if G has an independent set of size s by constructing G' and executing the supposed algorithm for finding a maximum 2-club. The running time would be dominated by the execution of this algorithm, which would take $2^{2^{o(\omega(G'))}}2^{o(n+m)}=2^{o(n+m)}$. We would therefore have a sub-exponential algorithm for MAXIMUM INDEPENDENT SET, which would contradict the ETH (Theorem 7).

Let us now describe the construction of G'. We assume without loss of generality that n and m are powers of 2 (otherwise we can take the union of G with an appropriate number of vertex-disjoint copies of K_2 and K_1 adjusting S as needed, while increasing the size of S by at most a constant factor). The vertices of S are partitioned into a clique S and an independent set S. More precisely:

- The vertices of the clique C are partitioned into three sets X, Y, Z, with $|X| = |Y| = 2 \log n + 1$ and $|Z| = 2 \log m$. Furthermore, we add to the clique two more vertices, call them z_0, z_1 .
- For each vertex $v \in V$ we construct a vertex a_v and place it in the independent set I of G'. Let $A = \{a_v \mid v \in V\}$.
- For each edge $e \in E$ with e = uv, with $u, v \in V$, we construct two vertices b_{eu} and b_{ev} and place them in the independent set I of G'. Let $B = \{b_{eu} \mid e \in E, u \in e\}$.

At this point the graph has a clique of size $4\log n + 2\log m + 4$ and an independent set of size n+2m and what remains is to describe the edges between C and I. Before we proceed, recall the basic fact that for all positive integers k we have $\binom{2k}{k} \geq 2^k$. We define three auxiliary functions f_X, f_Y, f_Z as follows. First $f_X: V \to 2^X$ is a function

We define three auxiliary functions f_X, f_Y, f_Z as follows. First $f_X: V \to 2^X$ is a function which assigns to each $v \in V$ a distinct set $f_X(v) \subseteq X$ such that $|f_X(v)| = \log n + 1$. Observe that since $|X| = 2\log n + 1$, there exist at least $\binom{2\log n + 1}{\log n + 1} = \binom{2\log n + 1}{\log n} \ge \binom{2\log n}{\log n} \ge 2^{\log n} = n$ distinct such sets, so it is possible to make f_X injective; furthermore we can construct such a function in time polynomial in n. Similarly, $f_Y: V \to 2^Y$ is a function that assigns to each $v \in V$ a distinct set $f_Y(v) \subseteq Y$ with $|f_Y(v)| = \log n + 1$. In a similar fashion, $f_Z: E \to 2^Z$ is a function which assigns to each $e \in E$ a distinct set $f_Z(e) \subseteq Z$ with $|f_Z(e)| = \log m$.

We are now ready to describe the remaining edges of G':

- 1. For each $v \in V$ make a_v adjacent to all of $f_X(v)$ and all of $f_Y(v)$.
- 2. For each $e \in E$ with e = uv, arbitrarily select one of u, v, say u, to be the first endpoint of e. Make b_{eu} adjacent to $\{z_0\} \cup f_Z(e) \cup (X \setminus f_X(u))$ and make b_{ev} adjacent to $\{z_1\} \cup (Z \setminus f_Z(e)) \cup (Y \setminus f_Y(v))$.

This completes the construction of G' and we set s' = s + m + |C|. Before proving that G' has a 2-club of size s' if and only if G has an independent set of size s, it will be helpful to make some basic observations about the independent set I of G'.

 \triangleright Claim 8. The only pairs of vertices of I which are at distance 3 in G' are of the following two forms:

- 1. b_{eu} , b_{ev} , for some $e \in E$ with e = uv
- **2.** b_{ev}, a_v , for some $e \in E$ with $v \in E$.

Proof. It is easy to see that pairs of the stated forms indeed have distance 3: b_{eu} , b_{ev} have disjoint neighborhoods in Z by construction; b_{ev} , a_v have disjoint neighborhoods because a_v has no neighbor in Z, and its neighborhood in X is $f_X(v)$ while b_{ev} is at most adjacent to $X \setminus f_X(v)$ (and similarly for Y).

What is more interesting is to observe that these are the only pairs of vertices from I at distance 3. To consider all other possible pairs we have the following cases:

- 1. Two vertices $a_v, a_u \in A$ are at distance 2. This can be seen as $|f_X(v)| = |f_X(u)| > \frac{|X|}{2}$ so $f_X(u)$ and $f_X(v)$ cannot be disjoint.
- 2. Two vertices $b_{ev}, b_{fu} \in B$, for two distinct edges $e, f \in E$ are at distance 2. This is easy to see if v, u are the first endpoints of the edges e, f, as they are both adjacent to z_0 (and similarly if they are both the second endpoints, they are both adjacent to z_1). Suppose then that v is the first endpoint of e and e the second endpoint of e. However, $f_Z(e) \neq f_Z(f)$, since f_Z is injective. Because $|f_Z(e)| = |f_Z(f)|$, there exist e with e is a common neighbor of e and e is a common neighbor of e.
- 3. A vertex $a_v \in A$ and a vertex $b_{eu} \in B$, with $u \neq v$ are at distance 2. Suppose without loss of generality (the other case being symmetric) that u is the first endpoint of e. Then b_{eu} is adjacent to $X \setminus f_X(u)$, therefore since all vertices of A have $\log n + 1$ neighbors in X, the only vertex of A that has no common neighbor with b_{eu} is a_u .

This concludes the proof of Claim 8.

Armed with Claim 8, we can now establish the correctness of the reduction. First, if G has an independent set S of size s, we select a 2-club S' in G' as follows: for each $v \in S$ we place a_v in S'; we place all of the clique in S'; and for each $uv \in E$ at least one of its endpoints, say u, is not in S, so we place the corresponding vertex b_{eu} in S'. Clearly we have a set of the desired size, that is s' = s + m + |C|. To see that it is a 2-club we observe that since all of the clique is in S' the distances between any two vertices are preserved, and we have not selected any of the forbidden pairs of Claim 8.

For the converse direction, suppose we have a 2-club S' of size s' in G'. We can assume without loss of generality that S' contains C because vertices of C are at distance at most 2 from all other vertices of the graph. Furthermore, we can modify S' so that it contains exactly m vertices of B as follows: if for some $e \in E$ with e = uv neither of b_{eu} , b_{ev} is contained in S', then we add b_{eu} to S' and remove a_u (if necessary), which thanks to Claim 8 gives another solution of at least the same size. Since for any edge $e \in E$ with e = uv we cannot have both b_{eu} and b_{ev} in S', as by Claim 8 these vertices are at distance 3, we conclude that S' contains s vertices of A, from which we extract a set S of G of size s. We claim that S is an independent set. Indeed, suppose $u, v \in S$ and $e = uv \in E$, then S' must contain b_{eu} or b_{ev} . Say without loss of generality that $b_{eu} \in S'$. Since $a_u \in S'$ (as we placed $u \in S$), by Claim 8 S' contains two vertices at distance 3, contradiction. We conclude that if G' has a 2-club of size s', then G has an independent set of size s.

4 An exact algorithm for Maximum 2-club in chordal graphs

We now turn our attention to chordal graphs with the aim of proposing an improved exact algorithm for Maximum 2-club for this class. Our algorithm relies on the simple observation that any 2-club that is not a clique must intersect a minimal separator (Observation 10). Then, by a careful analysis of the remaining possibilities, we observe that the problem can be reduced to that of finding a maximum-sized independent set in an arbitrary graph with the same number of vertices.

Throughout this section we let G = (V, E) be a chordal graph, and M be a maximum 2-club of G. We point out that the same results hold for inclusion-wise maximal 2-clubs. The following observation comes from the fact that a maximum clique can be found in linear time in chordal graphs through the enumeration of all minimal separators (see e.g. [17]).

- ▶ **Observation 9.** If M is a clique, it can be found in time O(n+m).
 - In the following, we will study the case in which M is not a clique.
- ▶ **Observation 10.** There exist $x, y \in M$ and a (x, y)-minimal separator S so that $S \cap M \neq \emptyset$.

Proof. As M is not a clique, there exist $x, y \in M$ so that $dist_M(x, y) \ge 2$. As M is a 2-club, we actually have $dist_M(x, y) = 2$, and there exists $z \in M$ so that (x, z, y) is an induced path in M. Then, for any (x, y)-separator $S, z \in S$ and thus $S \cap M \ne \emptyset$.

We now fix such a set S and provide further observations with respect to S.

▶ Lemma 11. The maximum 2-club M is included in the closed neighborhood of S in G.

Proof. By contradiction, let us assume that $z \in M \setminus N_G[S]$ exists. As S is a (x, y)-separator, x and y are in two different connected components of G - S. The vertex z is also in a connected component of G - S, so at least one among x, y are in a different component than z. Assume w.l.o.g. that z is not in the connected component of G - S containing x. We

claim that $dist_G(x, z) \geq 3$. Indeed if $dist_G(x, z) \leq 2$ there must be some path (x, w, z) in G, from the component C_x of G - S containing x to the component C_z containing z. This path necessarily intersects $N_G(C_x)$, and by Lemma 5 we have $N_G(C_x) = S$. Therefore $w \in S$, contradicting the assumption that z is not in the closed neighborhood of S. It remains that $dist_G(x, z) \geq 3$, and M is not a 2-club.

- ▶ **Definition 12** (bad pair). Let C be a connected component of G-S and consider two vertices $a, b \in C \cap N(S)$. We say that (a, b) is a bad pair if $dist_G(a, b) \ge 2$ and $N(a) \cap N(b) \cap S = \emptyset$.
- ▶ Lemma 13. Let $(a,b) \in M^2$ a bad pair. For all $c \in (N(a) \cap N(b)) \setminus S$, we have that $N(a) \cap S \subseteq N(c)$ and $N(b) \cap S \subseteq N(c)$.
- **Proof.** By contradiction, let us assume that there exists $a' \in N(a) \cap S$ so that $a' \notin N(c)$. As $b \in N(S)$ by definition of bad pairs, there exists $b' \in N(b) \cap S$, different from a'. If $b' \in N(c)$ then (a, a', b', c) is a chordless C_4 and otherwise, (a, a', b', b, c) is a chordless C_5 . Then, G cannot be chordal. It remains that $N(a) \cap S \subseteq N(c)$, and by symmetry also $N(b) \cap S \subseteq N(c)$.
- ▶ **Lemma 14.** Let a, b be two vertices in N[S]. If the distance between a and b in G[N[S]] is at least 3, then the distance between a and b in G is also at least 3.
- **Proof.** Since S is a clique (by Observation 6), note that the distance $dist_{N[S]}(a,b)$ between a and b in G[N[S]] is also at most 3.

Firstly, assume that a and b are in a same connected component C of G-S. Then the fact that the distance $dist_{N[S]}(a,b)=3$ implies that (a,b) is a bad pair. Suppose that $dist_G(a,b) \leq 2$. The only possibility would be that a and b have a common neighbor c in $V(G) \setminus N[S]$. Then by Lemma 13, $N(a) \cap S \subseteq N(c)$, thus $c \in N[S]$ – a contradiction.

It remains the case when a,b are in different components of G-S. But then if $dist_G(a,b) \leq 2$ the common neighbor of a and b on the (a,b)-path of length 2 is necessarily in S, contradicting $dist_{N[S]}(a,b) = 3$.

▶ **Definition 15** (auxiliary graph for S). Let us define the auxiliary graph H for the minimal separator S as follows: $V(H) = N_G[S]$ and for any pair of vertices $a, b \in N_G[S]$, $ab \in E(H)$ if and only if $dist_G(a, b) = 3$.

Again, recall that since S is a clique, the distance between any pair of vertices of $N_G[S]$ in G is at most 3. Also, by Lemma 14, being at distance 3 in G is the same as being at distance 3 in $G[N_G[S]]$. The following observation is simple but crucial in proving that the maximum (or maximal) 2-club M is actually a maximum (maximal) independent set of H.

▶ **Lemma 16.** Let I be an independent set of H, (a,b) a bad pair such that $a,b \in I$, and $c \in ((N_G(a) \cap N_G(b) \cap N_G(S)) \setminus I$. Then, $I \cup \{c\}$ is an independent set of H.

Proof. By contradiction, let us assume that there exists $d \in I$ so that $dist_G(c,d) \geq 3$. Since $a,b,d \in I$, we also have $dist_G(a,d) \leq 2$, $dist_G(b,d) \leq 2$ by construction of the auxiliary graph H (Definition 15). Then d is in the same connected component of G-S as a,b and c (otherwise we cannot have $dist_G(a,d) \leq 2$, $dist_G(b,d) \leq 2$ and $dist_G(c,d) \geq 3$ simultaneously according to Lemma 13). Also, (a,d) is a bad pair: we cannot have $dist_G(a,d) = 1$ because it would imply that $dist_G(c,d) \leq 2$ since $ac \in E(G)$, and we cannot have $dist_G(a,d) = 2$ and a,d have a common neighbor c' in S, because Lemma 13 applied to the bad pair (a,b) implies that $cc' \in E(G)$ thus $dist_G(c,d) \leq 2$. Similarly, (b,d) is a bad pair. Then there exist $e, f \in G$ so that (d,e,a) and (d,f,b) are induced paths, and e and f are in the same connected component as a,b,c and d (possibly e=f).

Assume that $e \neq f$. As G is chordal, there exists at least one of the chords (c, e) and (c, f) in the cycle (a, c, b, f, d, e). Then, $dist_G(c, d) = 2$, which contradicts our premise. If e = f then the cycle (a, c, b, f) must have a chord, and the only possibility is cf, entailing again the contradiction $dist_G(c, d) = 2$. This concludes the proof.

▶ **Lemma 17.** Let I be a maximal independent set of H. Then $S \subseteq I$ and I is a maximal 2-club of G among those contained in $N_G[S]$.

Proof. Since S is a clique in G (Observation 6), by maximality of I and definition of H we have $S \subseteq I$. Let us start by showing that I is a 2-club in G. To that aim, we prove that for any pair of vertices $(a,b) \in I^2$ it holds that $dist_I(a,b) \leq 2$. (In the remaining of the proof all distances are considered in G.) Let $(a,b) \in I^2$. If $a,b \in S$, $dist_I(a,b) = 1$ since S is a clique and we are done. If $a \in I \setminus S$ and $b \in S$, $dist_I(a,b) \leq 2$ by definition of H (recall that $V(H) = N_G[S]$ and that $a \in N_G[S]$).

Let us assume $a,b \in I \setminus S$. If (a,b) is not a bad pair (Definition 12), then either $dist_G(a,b) = 1$ or there exists $c \in S$ so that $c \in N_G(a) \cap N_G(b)$ and thus $dist_I(a,b) = 2$. If (a,b) is a bad pair, $N_G(a) \cap N_G(b) \cap S = \emptyset$. As $dist_G(a,b) \leq 2$ (by definition of H and the fact that $a,b \in I$), by Lemma 14 we also have $dist_{N_G[S]}(a,b) \leq 2$. Thus there exists $c \in N_G(a) \cap N_G(b) \cap N_G(S)$. If $c \notin I$, Lemma 16 shows that $I \cup \{c\}$ is an independent set of H. As I is maximal, this is not possible. Thus, $c \in I$, (a,c,b) is an induced path in I and $dist_I(a,b) = 2$.

To prove the maximality, assume there is some 2-club M of G contained in $N_G[S]$, strictly containing I. By construction of H, since any pair of vertices of M are at distance at most 2 in G[M] (and hence in G), we have that M is an independent set of H, contradicting the maximality of I.

The converse of Lemma 17 also holds.

▶ Lemma 18. Let M be a 2-club contained in $N_G[S]$. Then M is an independent set of the auxiliary graph H.

Proof. Since M is a 2-club any two vertices of M are at distance at most 2 in G, thus they are non-adjacent in H.

▶ **Theorem 2.** The maximum 2-club of a chordal graph G can be found in time $O^*(1.1996^n)$.

Proof. We use the following strategy to find a maximum 2-club in a chordal graph:

- 1. we enumerate all minimal separators of G, which can be done in time O(n+m) (see e.g. [17]);
- **2.** for every such separator S,
 - a. we construct the auxiliary graph H for S defined as $(N_G[S], E_H)$ where $ab \in E(H)$ iff $dist_G(a, b) \geq 3$;
 - **b.** we apply the algorithm of Xiao and Nagamochi [26] to compute a maximum independent set I_S of H in time $O(1.1996^n)$;
- 3. let I be the largest set I_S computed among all sets S.
- **4.** let K be the largest clique of G, which can be obtained in linear time, e.g. by [20].
- **5.** we output the largest set among I and K.

Observe that the set M returned by the algorithm is indeed a 2-club; this is trivial if the algorithm returns a clique K, and comes from Lemma 17 if the set returned by the algorithm is $I = I_S$ for some minimal separator S.

Let M' be a maximum 2-club of G, we need to prove that $|M| \ge |M'|$. If M' is a clique, then the maximum clique K constructed by the algorithm is at least of the same size and the conclusion follows. If M' is not a clique then it is contained in the neighborhood $N_G[S]$ of some minimal separator S of G by Lemma 11. Also by Lemma 18, it is an independent set of the auxiliary graph H for the minimal separator S. Therefore the set I_S constructed by the algorithm is of size at least M', and so is M.

We emphasise that the reduction of Lemma 17 can also be used to enumerate all maximal 2-clubs in a chordal graph in time $O^*(3^{\frac{n}{3}})$.

▶ **Theorem 3.** Chordal graphs have $O^*(3^{\frac{n}{3}})$ maximal 2-clubs, enumerable within the same running time.

Proof. Let G be a chordal graph. Maximal 2-clubs that are cliques are also maximal cliques of G. Their number is at most n and they are enumerable in linear time in chordal graphs [17].

It remains to enumerate maximal 2-clubs M that are not cliques. Recall that such 2-clubs intersect some minimal separator S of G (Lemma 11). Fix a minimal separator S, we count and enumerate the maximal 2-clubs M intersecting S. Construct the graph H associated to S as in Definition 15, clearly M is an independent set of H (Lemma 18). By Lemma 17 and the maximality of M, we actually must have that M is a maximal independent set of H. By a classic result of Moon and Moser [18], the graph H with at most n vertices has at most $3^{\frac{n}{3}}$ maximal independent sets, enumerable in time $O^*(3^{\frac{n}{3}})$.

Recall that G has at most n minimal separators which can be enumerated in linear time [17], completing the proof of the statement.

5 Split graphs with $\Omega^*(3^{\frac{n}{3}})$ maximum 2-clubs

In this section we provide a construction of (split) graphs that have $\Omega^*(3^{\frac{n}{3}})$ maximum 2-clubs, where $3^{\frac{n}{3}} \approx 1.4423^n$.

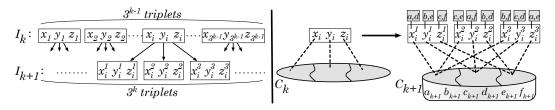
To that aim, we recursively construct the set of split graphs $(G_k = ((C_k, I_k), E_k))_{k \in \mathbb{N}^*}$, such that for all $k \in \mathbb{N}^*$, $|C_k| = 6k - 3$ and $|I_k| = 3^k$, so the graph G_k has $n = 3^k + O(k)$ vertices. Moreover the independent set I_k is partitioned into 3^{k-1} triplets. Then we will show that G_k has at least $3^{3^{k-1}}$ maximum (and inclusion-wise maximal) 2-clubs obtained by picking exactly one vertex from each triplet, plus the set C_k . This will lead to the $\Omega^*(3^{\frac{n}{3}})$ lower bound on the number of maximum (or inclusion-wise maximal) 2-clubs.

Construction of graphs G_k

We refer the reader to Figure 1 for an explanation of the construction.

- C_1 is a clique of size 3 and $I_1 = \{x_1, y_1, z_1\}$ is an independent set of size 3. We give each vertex of I_1 one neighbor in C_1 such that $(N(x_1), N(y_1), N(z_1))$ is a partition of C.
- $C_{k+1} = C_k \cup \{a_{k+1}, b_{k+1}, c_{k+1}, d_{k+1}, e_{k+1}, f_{k+1}\}$ with $\{a_{k+1}, b_{k+1}, c_{k+1}, d_{k+1}, e_{k+1}, f_{k+1}\}$ six new vertices. The independent set I_k is comprised of 3^k vertices split in 3^{k-1} distinct triplets (x_i, y_i, z_i) with $i \in [1, 3^{k-1}]$. To construct I_{k+1} , we triple the size of I_k by replacing each original vertex $v \in I_k$ with three copies v^1, v^2, v^3 . Thus, for each $i \in [1, 3^{k-1}]$, we transform the triplet (x_i, y_i, z_i) into three triplets $(x_i^1, y_i^1, z_i^1), (x_i^2, y_i^2, z_i^2)$ and (x_i^3, y_i^3, z_i^3) , keeping the invariant that I_{k+1} is formed of 3^k triplets (which can arbitrarily be renumbered from 1 to 3^k). Each edge uv of G_k with $u \in C_k$ and $v \in I_k$ will also be tripled, i.e., we put in E_{k+1} the three edges uv^1, uv^2 and uv^3 . Eventually, for all $i \in [1, 3^{k-1}]$ we add the following 18 edges to E_{k+1} :

```
 = (a_{k+1}, x_i^1), (a_{k+1}, y_i^2), (a_{k+1}, z_i^3) 
= (b_{k+1}, y_i^1), (b_{k+1}, z_i^2), (b_{k+1}, x_i^3) 
= (c_{k+1}, z_i^1), (c_{k+1}, x_i^2), (c_{k+1}, y_i^3) 
= (d_{k+1}, x_i^1), (d_{k+1}, z_i^2), (d_{k+1}, y_i^3) 
= (e_{k+1}, y_i^1), (e_{k+1}, x_i^2), (e_{k+1}, z_i^3) 
= (f_{k+1}, z_i^1), (f_{k+1}, y_i^2), (f_{k+1}, x_i^3)
```



- **Figure 1** Illustration of the construction. On the left side: each triplet from I_k is replaced by 3 triplets in I_{k+1} . On the right side: the neighborhoods (represented by dashed edges) of x_i , y_i and z_i form a partition of C_k . The clique C_{k+1} is made from C_k together with new vertices $a_{k+1}, b_{k+1}, c_{k+1}, d_{k+1}, e_{k+1}, f_{k+1}$. These 6 vertices of C_{k+1} are connected to the triplets of I_{k+1} as represented above the triplets (where subscripts are forgotten). In particular, the vertices a_{k+1} and d_{k+1} insure that x_i^1 is at distance at most 2 from all the other vertices in I_{k+1} except for y_i^1 and z_i^1 .
- ▶ Lemma 19. Let $k \geq 2$ be an integer, let $i \neq j$ be two integers in $[1,3^{k-1}]$, and let (x_i, y_i, z_i) and (x_j, y_j, z_j) denote the ith and the jth triplets of I_k . For all $u \in \{x_i, y_i, z_i\}$, $v \in \{x_j, y_j, z_j\}$, $N_{G_k}[u] \cap N_{G_k}[v] \neq \emptyset$.
- **Proof.** By construction of G_k and the set of 18 edges added between the six vertices $\{a_k, b_k, c_k, d_k, e_k, f_k\}$ of C_k and the triplets of I_k , we ensured that u, v have a common neighbor among $\{a_k, b_k, c_k, d_k, e_k, f_k\}$. See also Figure 1.
- ▶ Lemma 20. Let $k \in \mathbb{N}^*$. For all $i \in [1, 3^{n-1}]$, let (x_i, y_i, z_i) denote the ith triplet of I_k . For all $u, v \in \{x_i, y_i, z_i\}$, $N_{G_k}[u] \cap N_{G_k}[v] = \emptyset$.
- **Proof.** Let us prove this recursively. By definition of G_1 , $N_{G_1}[u] \cap N_{G_1}[v] = \emptyset$. Then, let us assume the premise is true for k. When tripling I_k to create I_{k+1} , we get $u^1, v^1, u^2, v^2, u^3, v^3$ from u and v. For $\ell \in [1,3]$, $N_{I_{k+1}}[u^\ell] = N_{I_{k+1}}[v^\ell] = \emptyset$ based on the construction of $(G_k)_{k \in \mathbb{N}^*}$. Indeed u and v have no common neighbor in C_k in graph G_k therefore u^ℓ and v^ℓ will have no common neighbor in $C_k \subseteq C_{k+1}$ in graph G_{k+1} . Amongst the six new vertices added to C_{k+1} , none is simultaneously a neighbor of u^ℓ and v^ℓ . Thus, $N_{G_{k+1}}[u^\ell] \cap N_{G_{k+1}}[v^\ell] = \emptyset$.
- ▶ **Lemma 21.** Let $k \in \mathbb{N}^*$. Let $A \subseteq I_k$ be a set of size $\frac{|I_k|}{3}$ such that one and only one vertex of each triplet of I_k is in A. Then, $C_k \cup A$ is a maximum 2-club of G_k .

Proof. Let us show that $C_k \cup A$ is a 2-club of G_k .

Let $u, v \in C_k \cup A$. If $u, v \in C_k$, $dist_{C_k \cup A}(u, v) = 1$ as C_k is a clique. If $u \in C_k$, $v \in A$, $dist_{C_k \cup A}(u, v) \leq 2$ as C_k is a clique and $N_{G_k}[v] \cap C_k \neq \emptyset$ by definition of G_k . If $u, v \in A$, we know by definition of A that u and v are not in the same triplet of I_k . Then u and v have a common neighbor in C_k (Lemma 19) and thus $dist_{C_k \cup A}(u, v) = 2$.

Now, let us prove that $C_k \cup A$ is maximum. Lemma 20 shows that for u, v in the same triplet of I_k , $dist_{G_k}(u, v) \geq 3$. Thus, there cannot exist a 2-club in G_k that has more vertices of I_k than 3^{k-1} (i.e. more than one by triplet). As for all $u \in G_k \setminus I_k = C_k$, $u \in C_k \cup A$, so $C_k \cup A$ is maximum.

▶ Theorem 4. For any $n \in \mathbb{N}$, there exists a split graph G of n vertices that contains $\Omega(3^{\frac{n}{3}}/\operatorname{poly}(n))$ distinct maximum (and inclusion-wise maximal) 2-clubs, for some fixed polynomial poly.

Proof. Let k be the maximum integer such that $3^k + 6k + 3 \le n$, in particular $3^k \ge n - O(\log n)$ hence $3^{k-1} \ge n/3 - O(\log n)$.

We focus on graph G_k , which has at most n vertices. (We can complete it with isolated vertices to obtain a graph with exactly n vertices, without diminishing the number of maximum 2-clubs.) Recall that I_k is composed of 3^{k-1} triplets (as $|I_k| = 3^k$), and by Lemma 21 there are $3^{3^{k-1}}$ maximum 2-clubs in G_k , by picking one vertex in each triplet plus the set C_k .

Plugging in the observation that $3^{k-1} \ge n/3 - O(\log n)$, we have that $3^{3^{k-1}}$ is $\Omega^*(3^{\frac{n}{3}})$. Thus we have constructed a family of graphs with $\Omega^*(3^{\frac{n}{3}})$ maximum (and hence, inclusion-wise maximal) 2-clubs.

▶ **Observation 22.** The exact same reasoning can be used with subsets of size x different than 3, to obtain split graphs with $\Omega^*(x^{\frac{n}{x}})$ maximum 2-clubs. But the function $f: x \mapsto x^{\frac{1}{x}}$ is greatest for x = 3 amongst all $x \in \mathbb{N}$.

6 Conclusion and open problems

We showed in this paper that the FPT algorithm for MAXIMUM 2-CLUB parameterized by vertex cover [13], with a double-exponential on vc(G), is essentially optimal under ETH. Note that [13] actually provides an algorithm with the same dependency on the treewidth of G, and since the latter is at most the vertex cover it cannot be essentially improved. A similar observation holds for the parameters vertex deletion distance to cographs and cluster graphs, respectively [14].

Consider problem MAXIMUM 2-CLUB, formulated as "does the input graph contain a 2-club of size at least ℓ ", with parameter ℓ . The problem is FPT, with a simple argument which actually yields a Turing kernel [24]: if the input graph G has a vertex x of degree at least $\ell-1$, then $N_G[x]$ is a trivial yes-instance. Therefore, we may assume that G has maximum degree $\ell-1$, and seek, for each vertex x, a 2-club containing x – therefore we only work in the graph $G[N_G[N_G[x]]]$, the second neighborhood of x. Because of the maximum degree being $\ell-1$, such a graph has $O(\ell^2)$ vertices, so the whole algorithm runs in time $O^*(2^{O(\ell^2)})$. We re-ask the following natural question:

▶ Question 1 ([14, 24]). Is there an algorithm for finding a 2-club of size at least ℓ , parameterized by ℓ , with running time $O^*(2^{O(\ell)})$?

When it comes to exact algorithms, we provided an algorithm for chordal graphs running in time $O^*(1.1996^n)$. For arbitrary graphs, the best known algorithm [24] runs in time $O^*(1.62^n)$ based on a simple and natural branching as follows. Let G^2 be the square of G, obtained from G by adding an edge between every pair of vertices at distance at most 2. If G^2 is a clique, then the whole graph is a 2-club. Otherwise, let x be a vertex and y be a non-neighbor of x in G^2 . Branch on G - x to find the largest 2-club not containing x, and also on G - y to find the largest 2-club containing x and hence not containing y. To follow the terminology of [8], this corresponds to a branching vector (2, 1): we reduce the number of vertices on which we can branch by 2 in the second case, since x is in the club and y is not, and by 1 in the first case when we simply discard x. This leads to the running time of $O^*(1.62^n)$. If, for example, x has two or more non-neighbors in G^2 , then when x is in the 2-club we exclude at least 2 other vertices and the branching vector becomes (3, 1), leading

to a better running time. In other words, the hardest instances are those where G^2 is a clique minus a matching. Not only such instances are easy to construct, but one can also rule out some naive ideas such as 'maybe in these instances, if y is the unique non-neighbor of x in G^2 , then any maximum 2-club contains at least one among x, y'. Therefore we ask:

▶ Question 2. Is there an exact algorithm for MAXIMUM 2-CLUB running in time $O^*(c^n)$ for some constant $c \le 1.61$?

Eventually, what is the maximum number of maximum (or inclusion-wise maximal) 2-clubs in an *n*-vertex graph?

▶ Question 3. Is there a constant $c > 3^{\frac{1}{3}} \simeq 1.4423$ such that for infinitely many $n \geq 0$ there are n-vertex graphs with at least c^n maximum (or inclusion-wise maximal) 2-clubs?

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